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PROPERTY PREDICTION FOR MULTICOMPONENT COMPOUNDS
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Principal Investigator: Dr. Nadezhda N.Kiselyova

Member of the research team:
Vitalii V.Petukhov

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Dr. Nadezhda Kiselyova

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Russian Academy of Sciences
Laboratory of Materials Sciences of Semiconductors
Leninsky Prospect, 49
Moscow 117334
Russia

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ABSTRACT

The new inorganic quaternary compounds most promising for searching for novell electro-optical (EO) materials are predicted on the base of the use of computer learning strategies. The basic working hypothesis of this investigation was that only compounds with acentric crystal space groups can have by EO properties. It is expected that new EO compounds will be similar in composition and crystal structure to already known compounds. The crystal chemical types were selected on the base of analysis of information of our DB on the properties of crystals of acousto-optical, electro-optical, and nonlinear-optical materials.

The results of predicting the crystal structure types at normal pressure and room temperature for the new compounds with composition of $A^{I}B^{II}(X^{VI}O)_4$ (A and B - any chemical elements; X - S, Cr, Mo, or W) are presented. Types considered were langbeinite and $K_2Zn_2(MoO_4)_3$. The predicted compounds with langbeinite structure hold the promise for searching for new EO materials. Prediction of the melilite crystal structure types at standard condiditions for the compounds with compositions $A^{II}_2B^{II}X^{IV}_2O_7$ (A and B - any chemical elements: X - Si, Ge, Sn, Ti, Zr, or Hf) and $A^{II}_2X^{IV}B^{III}_2O_7$ (A and B - any chemical elements; X - Si, Ge or Ti) was also carried out. Analysis of results shows: the great number of predictions of new melilites were obtained which hold the promise for searching for new EO materials. The results of predicting the crystal structure types at normal pressure and room temperature for the complicated borates with composition of $AD(BO_3)_4$ (A and D - any chemical elements; B - boron) are presented. Types considered were hantite, calcite and aragonite. Only compounds with acentric crystal structure type of hantite hold the promise for searching for new EO materials. For composition $A^{I}B^{II}C^{III}F_6$ (A = Li, Na, K, Rb, or Cs; B and C - any chemical elements) types considered included: colquirite ($LiCaAlF_6$), Na_2SiF_6, $RbNiCrF_6$, $CsAgFeF_6$, and trirutile. Analysis of results shows: the great number of predictions of new compounds with colquirite acentric crystal structure types and

Na_2SiF_6 were obtained, which hold the promise for searching for new EO materials. Predictions of the crystal structure types at standard conditions for the new compounds with composition $A_2^{I}B^{II}C^{III}F_7$ (A = Na or Ag; B and C - any chemical elements) were also carried out. Types considered included orthorhombic and trigonal weberites and fluorite. Analysis of results shows that many new compounds with crystal structure type of orthorhombic and trigonal weberites, which hold the promise for searching for new EO materials, were obtained.

The system of concept formation CONFOR supplied with system for discretization of initial components' features, which developed especially for predicting multi-component compounds, was used for computer learning and predicting. The main problems and prospects of the 'a priori' prediction of new multi-component inorganic compounds, which would have predefined properties, are discussed.

Subject terms (Key Words)
Concept formation, computer learning, discretization, prediction, inorganic compound, electro-optical, ferro-electric, colquirite, melilite, langbeinite, hantite, weberite, Na_2SiF_6.

FOREWORD

This final report was prepared by the above identified research team under EOARD Special Project SPC-96-4096 (Contract F61708-96-W0310). This work was carried out in close contact with researchers of the Materials Directorate, Wright Laboratory (USA) and V.M.Glushkov Institute of Cybernetics (Ukraine). We appreciate the management leadership of Dr. Steven R.LeClair. We thanks Prof. Viktor P.Gladun, Drs. Steven R.LeClair and Neonila D.Vaschenko, Prof. Allen G.Jackson, for their assistance. We also acknowledge the support provided by Dr.Jerry Sellers, of the EOARD, for enabling the interaction between ourselves and our colleagues from Wright Laboratory.

TABLE OF CONTENTS

1. INTRODUCTIONS

The goal of this investigation is to predict the new multi-element inorganic compounds which can be used for searching for the new electro-optical (EO) materials. The prediction is based on the use of computer learning strategies - a new approach to 'a priori' predicting of inorganic compounds that we develop from the early seventies.

The working hypothesis for these investigations is that the composition and crystal structure cause physical properties of a compound to a marked degree. It is expected that new EO compounds will be similar in composition and crystal structure to already known compounds. Therein, known classes of physico-chemical systems which exhibit peculiar EO properties provide the basis for the search for new compounds with interesting EO properties.

From our analysis of database (DB) on the properties of crystals of acousto-optical, electro-optical, and nonlinear-optical materials we have selected the promising phases to search for new EO compounds [1]. In this investigation we tried to predict the following compounds (Table 1.1).

Table 1.1

Promising Phases for Searching for New Electro-Optical Materials

Composition	Crystal structure type	Space group	Examples	Applications	Reference #
$A_2B_2C_3O_{12}$	Langbeinite	$P2_13$	$K_2Mg_2(SO_4)_3$ $Tl_2Cd_2(SO_4)_3$	EO	2-17
$A_2BC_2O_7$	Melilite	$P4(-)2_1m$	$Ba_2ZnGe_2O_7$ $Ba_2MgGe_2O_7$ $Ca_2MgSi_2O_7$ $Ca_2Al_2SiO_7$	EO Laser matrix	2
$ABCF_6$	Colquirite	P31c	$LiCaAlF_6$	EO Vacuum ultraviolet optics	2

Composition	Crystal structure type	Space group	Examples	Applications	Reference #
$ABCF_6$	Na_2SiF_6	P321	$LiMgAlF_6$	EO Vacuum ultraviolet optics	2
$AB_3C_4O_{12}$	Hantite	R32	$YAl_3B_4O_{12}$	EO "d"- and "f"- lasers	2
ABC_2F_7	Weberite	Imm2 or P3 21 1	Na_2MgAlF_7 Na_2MnFeF_7	EO "d"- lasers	2

A, B, C - chemical elements.

1.1. DEFINITIONS

Physical-chemical system - is a system (e.g., compound, or solid solution) which is formed from chemical elements.

Object - is a physical-chemical system which is described as a set of property (feature) values of the constituent elements.

Feature - is a property of the constituent component of the physical--chemical system.

Learning set - is a multidimensional array of feature values and a column vector of the desired property. Each row corresponds to some physical-chemical system already known, whose class is indicated by row position of the column vector.

Set for prediction - is a multidimensional array of feature values. Each row corresponds to some unknown physical-chemical system, whose class is necessary to predict.

Qualitative property - is an object or element property which can be described as a qualitative concept (e.g., multi-element system with compound formation or non-formation, crystal structure type, possibility of forming compounds of desired composition, and so on).

Quantitative property - is an object or element property which has a numeric values from some continuum (quasi-continuum) set of numbers (e.g., melting point, birefringence, index of refraction, and so on).

Concept - is a generalized model of some class of objects that is used for recognizing and generating models of specific elements of this class.

Pyramidal network - is an acyclic oriented graph having no vertices with one entering arc.

1.2. SYSTEM OF CONCEPT FORMATION C O N F O R

The program system CONFOR (CONcept FORmation) [18-20] serves as the basis for these investigations. The method of concept formation in pyramidal networks is used for discovery of complicated regularities in large scale data. It uses an especial data structure (pyramidal network) providing simplification of search operations and knowledge representation with using of feature values of negative objects (not belonging to the class under consideration) that provides discovery of more general regularities. The algorithm of concept formation in pyramidal network [18-20] is convergent and provides formation of the concepts dividing a training set of any complexity. Concepts are represented by collections of check vertices or by logical expressions. The concepts are analogs of complicated criteria which divide different classes of objects in multi-dimensional spaces of component features.

1.3. SYSTEM OF DISCRETIZATION

The problem of quantization (discretization) is a peculiarity of CONFOR and other logical algorithms of the computer learning method. These methods are usually applied to feature descriptions in which each feature has a finite number of values. Therefore at the stage of description formation ranges of numerical values are divided into nonintersecting subintervals each of which corresponds to one discrete value of a feature. Quantization is easy to solve if the classification has a qualitative nature (in case of the prediction of qualitative properties). For example, the types of the incomplete electronic shells have four gradation: s-, p-, d-, and f-shell. In the simplest cases, if quantitative properties are integer numbers in the narrow range, it makes sense to assign its gradation to each property value. For example, the number of electrons of the s-shell of the isolated atoms has three gradations: 0, 1 and 2.

It is important to note that the increase in the number of gradations

leads to the decrease in our ability to generalize about the properties of a concept and therein will necessitate an increase of the number of examples in the learning set. At the same time it is obvious that too small a number of gradations leads to the intersection of classes. When passing from binary physical-chemical system to multi-component systems (ternary, quaternary and so on), the program of discretization of component features becomes muchneeded tool. It is connected with complication of dividing criteria and small volume of learning sets.

The program of discretization of initial components' features was developed especially for predicting multi-component compounds [18]. An operation of discretization is fulfilled on the basis of comparison of distributions of learning set objects in scales of numerical values of features. Subintervals with the biggest density of object distribution as well as subinterwals containing separating values of the same class are choosen as discrete values of features. The program of discretization allowed to search the best gradations for component features in the case of predicting quaternary compounds. Moreover, the calculation time and size of logical expressions decreased.

Problem of the discretization program use was connected with vagueness of attribution of objects whose feature values do not fall within the obtained gradations. There are two ways of problem solution:

1). Elimination of such objects. This way is a good one if the volume of learning set is large. In the case of multi-component compound predicting this way leads to impossibility of recognition of practically the all set for prediction.

2). Gradation stretching by addition of missing values of predicted objects to the nearest interval. This way suffers from grave shortcoming: a possibility of erroneous prediction. But it is a sole way of predicting for complicated compounds. In these investigations we used this way.

2. RESULTS OF PREDICTION FOR MULTICOMPONENT COMPOUNDS

2.1. PREDICTION OF NEW COMPOUNDS OF COMPOSITION $A^{I}_{2}B^{II}_{2}(X^{VI}O)_{4}$

Compounds with the crystal structure of langbeinite $(K_2Mg_2(SO_4)_3$ (space group $P2_13$, $Z=4$) are of the doubtless interest for the search for new electro-optical, ferroelectric and luminescent materials [2-17]. As an example, linear electro-optical coefficients r_{41} are equ-

al to [3,3a] (10^{-8} C.G.S.E.) for: $K Mg (SO_4)_2$ - 1.2, $K Mn (SO_4)_2$ - 6, $(NH_4)_2 Mn (SO_4)_2$ - 1.59, $Tl Cd (SO_4)_2$ - 1.11, $Tl Mn (SO_4)_2$ - 6.3, $Rb Mn (SO_4)_2$ - 5.7, $Tl Mg (SO_4)_2$ - 1.8, $K Ni (SO_4)_2$ - 3. The langbeinites $Cs Cd (MoO_4)_2$ and $K Cd (SO_4)_2$ with piezoelectric coefficients $d_{14} = 5 * 10^{-12}$ and $d_{14} = 3.8 * 10^{-12}$ C/N can use in acoustoelectronics as delay lines and in nonlinear optics [4,13].

The following structural types: langbeinite and $K Zn (MoO_4)_2$ (space group $P2_1/c$, Z=4) are the most inherent for compounds with composition $A_2 B (XO_4)_3$. It is possible to allocate the three-dimensional skeletons of connected by common corners XO_4-tetrahedra and MO_6-octahedra in these compounds. The extent of association of the latter is the least one (separated octahedra) in the langbeinite structure and derivatives from it [5]. Just this feature of langbeinite structure causes the occurrence electro-optical properties.

Previously the efforts of the search for two-dimensional criteria which separated the different classes of compounds $A_2 B (XO_4)_3$ with various X were undertaken. In [4] it was proposed a structural map for classification of molybdates of mono- and bivalent elements. n - average of main quantum numbers and product of difference of electronegativities into ratio of ionic radii of elements A and B were used as coordinates of this map. The proposed structural map is enough good divided the compounds with structural types langbeinite and $K Zn (MoO_4)_2$. In [5] the langbeinite structure for X = Mo or W was considered in detail and mentioned that this structure with vast interstices is the most preferable for large monovalent cations: Rb^+, Cs^+ or Tl^+. It is reasonable because decreasing extent of condensation of structures of XO_4-tetrahedra and MO_6-octahedra with increasing size of monovalent cations causes, on the one hand, greater and grea-

ter isolation of MO_6 -octahedra, and on the other - decreasing dimension of their polyhedral structures connected with gradual transformation: skeleton-> layer-> tape. Thus it was mentioned [5] that prediction of crystal structure type for compounds of composition $A_2B_2(XO_4)_3$ account must be taken of the chemical peculiarities of bivalent cations and anions X besides size factor for monovalent cations.

2.1.1. DATA FOR COMPUTER LEARNING

The data for computer learning was extracted from our the cardfile on quaternary inorganic compound properties. On the base of analysis of these data it may be concluded that only compounds $A_2B_2(XO_4)_3$ with X= = S, Cr, Mo, or W can crystallize in langbeinite structure. Therefore this structure at room state and normal pressure was predicted only for sulfates, chromates, molybdates, and tungstates. The table 2.1.1.1 contains a learning set.

Table 2.1.1.1

Learning Set for Prediction of the Crystal Structure Type of Compounds with Composition $A_2B_2(XO_4)_3$

Composition	Crystal type	Space group
K2Mg2(SO4)3	langbeinite	
Rb2Mg2(SO4)3	langbeinite	
Rb2Mg2(MoO4)3	langbeinite	
Rb2Mg2(WO4)3	langbeinite	
Cs2Mg2(MoO4)3	langbeinite	
Tl2Mg2(MoO4)3	langbeinite	
K2Ca2(SO4)3	langbeinite	
K2Mn2(SO4)3	langbeinite	
K2Co2(SO4)3	langbeinite	
K2Ni2(SO4)3	langbeinite	
K2Zn2(SO4)3	langbeinite	
K2Cd2(SO4)3	langbeinite	
Cs2Ca2(SO4)3	langbeinite	
Rb2Mn2(SO4)3	langbeinite	
Tl2Mn2(SO4)3	langbeinite	
Rb2Cd2(SO4)3	langbeinite	
Tl2Cd2(SO4)3	langbeinite	
Rb2Mn2(CrO4)3	langbeinite	
Rb2Mn2(MoO4)3	langbeinite	

Composition	Crystal type	Space group
Cs2Mn2(MoO4)3	langbeinite	
Tl2Mn2(MoO4)3	langbeinite	
Rb2Co2(MoO4)3	langbeinite	
Cs2Co2(MoO4)3	langbeinite	
Rb2Ni2(MoO4)3	langbeinite	
Cs2Ni2(MoO4)3	langbeinite	
Tl2Ni2(MoO4)3	langbeinite	
Cs2Cd2(MoO4)3	langbeinite	
Tl2Fe2(SO4)3	langbeinite	
Tl2Co2(SO4)3	langbeinite	
K2Mg2(MoO4)3	K2Zn2(MoO4)3	
K2Co2(MoO4)3	K2Zn2(MoO4)3	
K2Ni2(MoO4)3	K2Zn2(MoO4)3	
K2Cu2(MoO4)3	K2Zn2(MoO4)3	
K2Zn2(MoO4)3	K2Zn2(MoO4)3	
Rb2Zn2(MoO4)3	K2Zn2(MoO4)3	
Tl2Zn2(MoO4)3	K2Zn2(MoO4)3	
Na2Zn2(MoO4)3	Li2Fe2(MoO4)3	P2(1)/c, Z=4
K2Mg2(WO4)3		P2(1)2(1)2(1), Z=4
K2Mn2(MoO4)3		Pcca, Z=8
Tl2Co2(MoO4)3		tetragonal
Rb2Cd2(MoO4)3		P2(1)2(1)2(1), Z=2
Na2SO4-CaSO4	Without compound A2B2(XO4)3	
Na2SO4-MnSO4	Without compound A2B2(XO4)3	
Na2SO4-CoSO4	Without compound A2B2(XO4)3	
Na2SO4-NiSO4	Without compound A2B2(XO4)3	
Na2SO4-CuSO4	Without compound A2B2(XO4)3	
Na2SO4-SrSO4	Without compound A2B2(XO4)3	
Na2SO4-CdSO4	Without compound A2B2(XO4)3	
Na2SO4-BaSO4	Without compound A2B2(XO4)3	
Na2MoO4-CaMoO4	Without compound A2B2(XO4)3	
Na2WO4-CaWO4	Without compound A2B2(XO4)3	
Na2CrO4-PbCrO4	Without compound A2B2(XO4)3	
Na2MoO4-SrMoO4	Without compound A2B2(XO4)3	
Na2WO4-SrWO4	Without compound A2B2(XO4)3	
Na2MoO4-BaMoO4	Without compound A2B2(XO4)3	
Na2MoO4-PbMoO4	Without compound A2B2(XO4)3	
Na2WO4-CdWO4	Without compound A2B2(XO4)3	
Na2WO4-PbWO4	Without compound A2B2(XO4)3	
Cs2SO4-MgSO4	Without compound A2B2(XO4)3	
Tl2SO4-CaSO4	Without compound A2B2(XO4)3	
Rb2SO4-BaSO4	Without compound A2B2(XO4)3	

Composition	Crystal type	Space group
Tl2SO4-SrSO4	Without compound A2B2(XO4)3	
Cs2SO4-BaSO4	Without compound A2B2(XO4)3	
Tl2SO4-BaSO4	Without compound A2B2(XO4)3	
Rb2MoO4-PbMoO4	Without compound A2B2(XO4)3	
Rb2WO4-PbWO4	Without compound A2B2(XO4)3	
Cs2WO4-PbWO4	Without compound A2B2(XO4)3	

2.1.2. SELECTION OF FEATURES

On the basis of physical-chemical grounds two sets of chemical elements features and set of simlpe oxides feature were selected for the description of these systems.

2.1.2.1. FEATURE SET 2.1.1

The first feature set (feature set 2.1.1) includes information about the number of electrons in energy shells of isolated atoms and Shannon effective ionic radii of elements A (C.N.=12), B (C.N.=6) or X (C.N.=4) in the compound of composition $A_2B_2(XO_4)_3$ (57 features for each compound). The grouping of energy shell information (hereafter referred to as gradation) corresponds to the number of electrons for each shell. In this task and subsequent text data about the all element and single compounds were extracted from our cardfiles of elements' and binary compounds' properties. The quasi-continuous properties - the ionic radii - were divided (quantized) using the special program of discretization [18]. Table 2.1.2.1.1 contains the gradations for Feature Set 2.1.1.

Table 2.1.2.1.1

Gradations for Feature Set 2.1.1

Feature	Gradation	Feature	Gradation
	A-element		
3s-shell		5s-shell	
s1	s3_1_1	s0	s5_0_1
s2	s3_2_1	s1	s5_1_1
3p-shell		s2	s5_2_1
p0	p3_0_1	5p-shell	
p6	p3_6_1	p0	p5_0_1

Feature	Gradation	Feature	Gradation
3d-shell		p6	p5_6_1
d0	d3_0_1	5d-shell	
d10	d3_10_1	d0	d5_0_1
4s-shell		d10	d5_10_1
s0	s4_0_1	6s-shell	
s1	s4_1_1	s0	s6_0_1
s2	s4_2_1	s1	s6_1_1
4p-shell		s2	s6_2_1
p0	p4_0_1	6p-shell	
p6	p4_6_1	p0	p6_0_1
4d-shell		p1	p6_1_1
d0	d4_0_1	Ionic	
d10	d4_10_1	radius, A	
4f-shell		[1.39-1.4047]	R1_1
f0	f4_0_1	(1.6301-1.6546]	R2_1
f14	f4_14_1	(1.6938-1.733]	R3_1
		(1.8702-1.88]	R4_1
	B-element		
3s-shell		5s-shell	
s2	s3_2_2	s0	s5_0_2
3p-shell		s2	s5_2_2
p0	p3_0_2	5p-shell	
p6	p3_6_2	p0	p5_0_2
3d-shell		p6	p5_6_2
d0	d3_0_2	5d-shell	
d10	d3_10_2	d0	d5_0_2
4s-shell		d10	d5_10_2
s0	s4_0_2	6s-shell	
s1	s4_1_2	s0	s6_0_2
s2	s4_2_2	s2	s6_2_2
4p-shell		6p-shell	
p0	p4_0_2	p0	p6_0_2
p6	p4_6_2	p2	p6_2_2
4d-shell		Ionic	
d0	d4_0_2	radius, A	
d5	d4_5_2	[0.45-0.7296]	R1_2
d6	d4_6_2	(0.7296-0.7362]	R2_2
d7	d4_7_2	(0.7362-0.7428]	R3_2
d8	d4_8_2	(0.7428-0.7626]	R4_2
d10	d4_10_2	(0.7626-0.8]	R4_2
4f-shell		[0.822-0.86]	R5_2
f0	f4_0_2	[0.9408-0.9672]	R6_2

Feature	Gradation	Feature	Gradation
f14	f4_14_2	[0.9804-1.02]	R7_2
		[1.17-1.2048]	R8_2
		[1.3368-1.35]	R9_2
	X-element		
3p-shell		5s-shell	
p4	p3_4_3	s0	s5_0_3
p6	p3_6_3	s1	s5_1_3
3d-shell		s2	s5_2_3
d0	d3_0_3	5p-shell	
d5	d3_5_3	p0	p5_0_3
d10	d3_10_3	p6	p5_6_3
4s-shell		5d-shell	
s0	s4_0_3	d0	d5_0_3
s1	s4_1_3	d4	d5_4_3
s2	s4_2_3	d10	d5_10_3
4p-shell		6s-shell	
p0	p4_0_3	s0	s6_0_3
p6	p4_6_3	s2	s6_2_3
4d-shell		Ionic	
d0	d4_0_3	radius, A	
d5	d4_5_3	[0.12-0.129]	R1_3
d10	d4_10_3	[0.255-0.28]	R2_3
4f-shell		[0.405-0.417]	R3_3
f0	f4_0_3	(0.417-0.43]	R4_3
f14	f4_14_3		

2.1.2.2. FEATURE SET 2.1.2

The second feature set (feature set 2.1.2) includes the following information: the first three ionization potentials, the electronegativities by Pauling, the entropies of the individual substances at 298 K, the isobaric thermal capacities at 298 K, the temperatures and the heats of melting and boiling, Debye (characteristic) temperatures, the energies of the crystal lattice, the ionic radii by Shannon, the ratio of the atomic number to the average atomic mass for atoms of elements A, B and X. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.1.2.2.1 contains the gradations for Feature Set 2.1.2.

Table 2.1.2.2.1

Gradations for Feature Set 2.1.2

Feature	Gradation	Feature	Gradation
	A-element		
First ionization potential, eV		Boiling point, K	
[3.89391-3.960342]	I1_1_1	[945-985]	Tb_1_1
[4.137493-4.226068]	I1_2_1	[1017-1057]	Tb_2_1
[4.314644-4.40322]	I1_3_1	[1137-1177]	Tb_3_1
[5.111825-5.2004]	I1_4_1	[1721-1745]	Tb_4_1
[6.041869-6.1083]	I1_5_1	Heat of melting, kJ/mol	
Second ionization potential, eV		[2.096-2.24804]	Hm_1_1
		[2.29148-2.40008]	Hm_2_1
[20.43-21.23571]	I2_1_1	[2.57384-2.66072]	Hm_3_1
[22.84713-23.92141]	I2_2_1	[4.22456-4.268]	Hm_4_1
[26.60711-27.94996]	I2_3_1	Heat of boiling, kJ/mol	
[31.1728-32.24708]	I2_4_1		
[46.74986-47.287]	I2_5_1	[76.442-83.27484]	Hb_1_1
Third ionization potential, eV		[87.17932-91.0838]	Hb_2_1
		[104.7495-109.6301]	Hb_3_1
[29.85-31.1031]	I3_1_1	[172.1018-174.054]	Hb_4_1
[32.7739-34.4447]	I3_2_1	Energy of the crystal lattice, -6 E*10 J/kg*mol	
[38.6217-40.2925]	I3_3_1		
[45.3049-46.9757]	I3_4_1		
[70.36691-71.62]	I3_5_1		
Electronegativity		[79-82.114]	E_1_1
[0.7-0.733]	X_1_1	[84.19-92.494]	E_2_1
[0.777-0.832]	X_2_1	[107.026-111.178]	E_3_1
[0.876-0.931]	X_3_1	[179.686-182.8]	E_4_1
[1.767-1.8]	X_4_1	Debye temperature, K	
Entropies of individual substances at 298 K kJ/kg*mol*K		[39.2-42.824]	Td_1_1
		[52.488-58.528]	Td_2_1
		[87.52-93.56]	Td_3_1
[51.296-52.31396]	S_1_1	[156.376-160]	Td_4_1
[63.1722-65.54744]	S_2_1	Ratio of the atomic number to the average atomic mass	
[75.72704-77.42364]	S_3_1		
[84.21004-85.228]	S_4_1		
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		[0.4-0.4027]	NM_1_1
		[0.4081-0.4126]	NM_2_1
[26.317-26.49274]	Cp_1_1	[0.4288-0.4324]	NM_3_1
[28.13298-28.3673]	Cp_2_1	[0.4774-0.4819]	NM_4_1

Feature	Gradation	Feature	Gradation
[29.42174-29.71464]	Cp_3_1	[0.4873-0.49]	NM_5_1
[30.88624-31.17914]	Cp_4_1	Ionic radius, A	
[31.99926-32.175]	Cp_5_1	[1.39-1.4047]	Rs_1_1
Melting point, K		[1.6301-1.6546]	Rs_2_1
[301.67-318.1298]	Tm_1_1	[1.6938-1.733]	Rs_3_1
[329.103-342.8195]	Tm_2_1	[1.8702-1.88]	Rs_4_1
[364.7659-378.4824]	Tm_3_1		
[570.5134-576]	Tm_4_1		
	B-element		
First ionization potential, eV		Boiling point, K	
		[630-1105.36]	Tb_1_2
[5.21166-5.337139]	I1_1_2	[1149.167-1236.781]	Tb_2_2
[5.588098-5.79723]	I1_2_2	[1324.396-1412.01]	Tb_3_2
[6.048188-6.254]	I1_3_2	[1593-1718.659]	Tb_4_2
[6.74-7.428459]	I1_4_2	(1718.659-1828.176]	Tb_5_2
(7.428459-7.721244]	I1_5_2	[1959.597-2178.632]	Tb_6_2
(7.721244-7.846724]	I1_6_2	[2310.053-2397.667]	Tb_7_2
(7.846724-7.88855]	I1_6_2	[2745-2950]	Tb_8_2
(7.88855-8.336]	I1_8_2	[3098.579-3164.29]	Tb_9_2
[8.93421-9.101516]	I1_9_2	(3164.29-4100]	Tb_10_2
[9.268821-10.4376]	I1_10_2	Heat of melting, kJ/mol	
Second ionization potential, eV		[2.295-5.158496]	Hm_1_2
[10.004-10.31267]	I2_1_2	[5.921207-6.5568]	Hm_2_2
[10.72423-11.24]	I2_2_2	[6.811038-7.192394]	Hm_3_2
[11.65024-12.18]	I2_3_2	(7.192394-7.57375]	Hm_4_2
[13.58-15.25139]	I2_4_2	[8.082224-8.463579]	Hm_5_2
[15.45717-15.935]	I2_5_2	(8.463579-9.21096]	Hm_6_2
[16.07451-16.5]	I2_6_2	[10.467-12.552]	Hm_7_2
[16.69185-17.30919]	I2_7_2	[12.65849-13.29409]	Hm_8_2
[17.72075-18.13231]	I2_8_2	[13.54832-15.062]	Hm_9_2
(18.13231-18.76]	I2_9_2	[16.0907-16.736]	Hm_10_2
[19.43-20.293]	I2_10_2	[17.10765-31.81968]	Hm_11_2
Third ionization potential, eV		Heat of boiling, kJ/mol	
[24.9-31.63988]	I3_1_2	[59.229-107.8633]	Hb_1_2
(31.63988-33.1247]	I3_2_2	(107.8633-121.6705]	Hb_2_2
(33.1247-35.5994]	I3_3_2	[138.2392-149.2849]	Hb_3_2
(35.5994-36.58928]	I3_4_2	(149.2849-165.8536]	Hb_4_2
(36.58928-37.08422]	I3_5_2	(165.8536-174.1379]	Hb_5_2
(37.08422-38.56904]	I3_6_2	(174.1379-185.1836]	Hb_6_2
(38.56904-41.04374]	I3_7_2	[223.8438-234.8896]	Hb_7_2

Feature	Gradation	Feature	Gradation
[42.03362-44.01338]	I3_8_2	[295.6412-314.637]	Hb_8_2
[49.95266-51.93242]	I3_9_2	[339.741-356.3929]	Hb_9_2
[78.65918-153.9]	I3_10_2	[361.9158-510.448]	Hb_10_2
Electronegativity		Energy of the	
[0.9-0.9299999]	X_1_2	crystal lattice,	
[0.97-1.1]	X_2_2	-6	
[1.18-1.23]	X_3_2	E*10 J/kg*mol	
[1.47-1.52]	X_4_2	[116-125.42]	E_1_2
[1.58-1.63]	X_5_2	(125.42-137.98]	E_2_2
[1.69-1.73]	X_6_2	[144.26-156.82]	E_3_2
[1.77-1.82]	X_7_2	(156.82-185.08]	E_4_2
[1.88-2.2]	X_8_2	(185.08-200.78]	E_5_2
Entropies of		[282.42-294.98]	E_6_2
individual		[321.6-364.7]	E_7_2
substances at 298 K		[390-414.3]	E_8_2
kJ/kg*mol*K		[420.58-510]	E_9_2
[9.498-28.911]	S_1_2	Debye	
[29.1845-32.8394]	S_2_2	temperature, K	
(32.8394-34.0577]	S_3_2	[75-106.16]	Td_1_2
[37.656-42.5858]	S_4_2	[121.04-139.64]	Td_2_2
[50.7078-52.7383]	S_5_2	[184.28-199.16]	Td_3_2
[55.1749-56.7993]	S_6_2	[214.04-233]	Td_4_2
[61.6725-63.2969]	S_7_2	[275-314.48]	Td_5_2
[66.5457-79.898]	S_8_2	[336.8-370]	Td_6_2
Isobaric thermal		[380-414.92]	Td_7_2
capacity at 298 K,		[430-1160]	Td_8_2
kJ/kg*mol*K		Ratio of the	
[16.443-24.5442]	Cp_1_2	atomic number	
[24.7626-24.9446]	Cp_2_2	to the average	
(24.9446-25.1208]	Cp_3_2	atomic mass	
[25.345-25.527]	Cp_4_2	[0.4-0.403]	NM_1_2
[25.857-26.0002]	Cp_5_2	[0.407-0.41226]	NM_2_2
(26.0002-26.1458]	Cp_6_2	[0.428-0.44]	NM_3_2
[26.2186-26.3642]	Cp_7_2	[0.45-0.462]	NM_4_2
(26.3642-26.5462]	Cp_8_2	[0.468-0.472]	NM_5_2
[26.6918-26.8738]	Cp_9_2	[0.478-0.482]	NM_6_2
[27.9658-28.075]	Cp_10_2	[0.488-0.492]	NM_7_2
Melting point, K		[0.498-0.5]	NM_8_2
[234.29-630.54]	Tm_1_2	Ionic radius, A	
[679.26-727.98]	Tm_2_2	[0.45-0.7296]	Rs_1_2
[898.5-959.4]	Tm_3_2	(0.7296-0.7362]	Rs_2_2
[983.76-1069.02]	Tm_4_2	(0.7362-0.7428]	Rs_3_2
[1093.38-1210.4]	Tm_5_2	(0.7428-0.7626]	Rs_4_2

Feature	Gradation	Feature	Gradation
[1336.98-1385.7]	Tm_6_2	(0.7626-0.8]	Rs_5_2
[1531.86-1592.76]	Tm_7_2	[0.822-0.86]	Rs_6_2
[1714.56-1799.82]	Tm_8_2	[0.9408-0.9672]	Rs_7_2
(1799.82-2190]	Tm_9_2	[0.9804-1.02]	Rs_8_2
		[1.17-1.2048]	Rs_9_2
		[1.3368-1.35]	Rs_10_2
	X-element		
First ionization potential, eV		Boiling point, K	
[6.766-6.873821]	I1_1_3	[717.7-1285]	Tb_1_3
[7.017582-7.197285]	I1_2_3	[2862.943-3072.235]	Tb_2_3
[7.916092-8.059855]	I1_3_3	[4746.571-5008.186]	Tb_3_3
[9.01-10.36004]	I1_4_3	[5845.354-5950]	Tb_4_3
Second ionization potential, eV		Heat of melting, kJ/mol	
[16.16-16.37534]	I2_1_3	[1.41095-5.44284]	Hm_1_3
(16.37534-16.66246]	I2_2_3	[17.50082-22.44387]	Hm_2_3
[17.52382-18.6]	I2_3_3	[35.66456-38.06832]	Hm_3_3
[21.16-23.338]	I2_4_3	[59.70218-61.505]	Hm_4_3
Third ionization potential, eV		Heat of boiling, kJ/mol	
[24-24.3249]	I3_1_3	[194.686-254.1653]	Hb_1_3
[26.9241-27.96]	I3_2_3	[328.5345-355.095]	Hb_2_3
[30.7146-31.2561]	I3_3_3	[567.5786-594.139]	Hb_3_3
[34.5051-34.83]	I3_4_3	[753.5017-769.438]	Hb_4_3
Electronegativity		Energy of the crystal lattice, $E*10^{-6}$ J/kg*mol	
[1.6-1.627]	X_1_3	[199.5-243.46]	E_1_3
[1.681-1.726]	X_2_3	[325.3-352.58]	E_2_3
[1.78-2.1]	X_3_3	[639.02-666.3]	E_3_3
[2.4-2.5]	X_4_3	[884.54-905]	E_4_3
Entropies of individual substances at 298 K kJ/kg*mol*K		Debye temperature, K	
[23.64-23.91111]	S_1_3	[89-192.15]	Td_1_3
[28.42961-28.88146]	S_2_3	[394.65-414.9]	Td_2_3
[31.7733-32.13478]	S_3_3	[463.5-479.7]	Td_3_3
[32.49626-49.73918]	S_4_3	[576.9-585]	Td_4_3
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		Ratio of the atomic number to the average atomic mass	
[22.60872-22.65973]	Cp_1_3		

Feature	Gradation	Feature	Gradation
[23.30584-23.39085]	Cp_2_3	[0.4-0.41]	NM_1_3
[24.03695-24.10497]	Cp_3_3	[0.43-0.442]	NM_2_3
[24.27499-25.74882]	Cp_4_3	[0.458-0.462]	NM_3_3
Melting point, K		[0.498-0.5]	NM_4_3
[392-930]	Tm_1_3	Ionic radius, A	
[2077.04-2242.24]	Tm_2_3	[0.12-0.129]	Rs_1_3
[2836.96-2969.12]	Tm_3_3	[0.255-0.28]	Rs_2_3
[3629.92-3696]	Tm_4_3	[0.405-0.417]	Rs_3_3
		(0.417-0.43]	Rs_4_3

2.1.2.3. FEATURE SET 2.1.3

The third set of properties of simple oxides (feature set 2.1.3) includes the following information of simple oxides AO_2, BO and XO_3 : the melting and boiling (only for BO and XO_3) points, standard enthalpy of formation, standard isobaric thermal capacities, standard entropies, standard Gibbs energy, effective ionic radii of correspoding cations by Shannon. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.1.2.3.1 contains the gradations for Feature Set 2.1.3.

Table 2.1.2.3.1

Gradations for Feature Set 2.1.3
(Properties of Simple Oxides)

Feature	Gradation	Feature	Gradation
	AO_2		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
[40-42.022]	H_1_1	[8.9-9.191]	Cp_1_1
[79.766-84.484]	H_2_1	[16.951-17.339]	Cp_2_1
[85.832-88.528]	H_3_1	(17.339-17.63]	Cp_3_1
[106.052-107.4]	H_4_1	(17.63-17.921]	Cp_4_1
		[18.309-18.6]	Cp_5_1

Feature	Gradation	Feature	Gradation
Standard Gibbs energy for simple oxides, kcal/mol		Melting point of simple oxides, K	
[40-41.50375]	G_1_1	[768-799.2]	Tm_1_1
[70.57625-75.0875]	G_2_1	[830.4-869.4]	Tm_2_1
[79.0975-81.1025]	G_3_1	[994.2-1033.2]	Tm_3_1
[89.12251-90.125]	G_4_1	[1532.4-1548]	Tm_4_1
Standard entropy for corresponding simple oxides, cal/mol*K		Ionic radii, A	
[17.7-18.222]	So_1_1	[1.39-1.4047]	Rs_1_1
[22.746-24.312]	So_2_1	[1.6301-1.6546]	Rs_2_1
[29.532-30.402]	So_3_1	[1.6938-1.733]	Rs_3_1
[34.578-35.1]	So_4_1	[1.8702-1.88]	Rs_4_1
	BO		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
[17-42.1121]	H_1_2	[6.11-9.22]	Cp_1_2
[48.8963-54.5498]	H_2_2	[9.5365-9.7089]	Cp_2_2
(54.5498-62.4647]	H_3_2	[9.967501-10.0968]	Cp_3_2
(62.4647-65.8568]	H_4_2	(10.0968-10.2261]	Cp_4_2
[81.6866-86.2094]	H_5_2	[10.3123-10.7002]	Cp_5_2
[90.73219-103.2]	H_6_2	(10.7002-11.045]	Cp_6_2
[125.7-133.6988]	H_7_2	[11.1312-11.3467]	Cp_7_2
[138.2216-142.7444]	H_8_2	[11.8639-12.0363]	Cp_8_2
(142.7444-146.1365]	H_9_2	[13.0707-13.2]	Cp_9_2
[148.3979-151.79]	H_10_2	Melting point of simple oxides, K	
Standard Gibbs energy for simple oxides, kcal/mol		[780-1216.42]	Tm_1_2
		[1484.38-1560.94]	Tm_2_2
		[1599.22-1694.92]	Tm_3_2
		[2039.44-2154.28]	Tm_4_2
[14.015-34.31845]	G_1_2	[2192.56-2230.84]	Tm_5_2
[43.38365-47.91625]	G_2_2	(2230.84-2288.26]	Tm_6_2
(47.91625-58.1146]	G_3_2	(2288.26-2345.68]	Tm_7_2
(58.1146-61.51405]	G_4_2	[2805.04-2900.74]	Tm_8_2
[75.11185-79.64445]	G_5_2	(2900.74-2977.3]	Tm_9_2
[84.17705-96.229]	G_6_2	[3015.58-3073]	Tm_10_2

Feature	Gradation	Feature	Gradation
[118.69-127.2367]	G_7_2	Boiling point of	
[131.7693-135.1688]	G_8_2	simple oxides, K	
(135.1688-138.599]	G_9_2	[1746-1809.81]	Tb_1_2
[140.8345-144.234]	G_10_2	[2235.21-2320.29]	Tb_2_2
Standard entropy		[3086.01-3171.09]	Tb_3_2
for corresponding		[3809.19-4283]	Tb_4_2
simple oxides,		Ionic radii, A	
cal/mol*K		[0.45-0.7296]	Rs_1_2
[3.29-6.7919]	So_1_2	(0.7296-0.7362]	Rs_2_2
[8.03-9.3671]	So_2_2	(0.7362-0.7428]	Rs_3_2
[10.0109-10.3328]	So_3_2	(0.7428-0.7626]	Rs_4_2
(10.3328-10.6547]	So_4_2	(0.7626-0.8]	Rs_5_2
[12-13.1226]	So_5_2	[0.822-0.86]	Rs_6_2
(13.1226-13.5]	So_6_2	[0.9408-0.9672]	Rs_7_2
[14.3029-14.6248]	So_7_2	[0.9804-1.02]	Rs_8_2
(14.6248-14.9467]	So_8_2	[1.1718-1.2048]	Rs_9_2
[16.2343-16.6635]	So_9_2	[1.3368-1.35]	Rs_10_2
[16.8-17.2]	So_10_2		
	XO 3		
Standard enthalpy		Standard isobaric	
of formation for		thermal capacity	
corresponding		for simple oxides,	
simple oxides,		cal/mol*K	
kcal/mol		[17.65-17.9035]	Cp_1_3
[104.92-107.8144]	H_1_3	(17.9035-18.664]	Cp_2_3
[138.688-143.512]	H_2_3	[42.493-43]	Cp_3_3
[176.3152-180.1744]	H_3_3	Melting point of	
[199.4704-201.4]	H_4_3	simple oxides, K	
Standard Gibbs		[289.89-333.5733]	Tm_1_3
energy		[450.0621-508.3065]	Tm_2_3
for simple oxides,		[1032.506-1105.312]	Tm_3_3
kcal/mol		[1716.878-1746]	Tm_4_3
[89.9-92.68004]	G_1_3	Boiling point of	
[120.4804-125.1138]	G_2_3	simple oxides, K	
[158.4743-162.181]	G_3_3	[317.9-351.203]	Tb_1_3
[180.7146-182.568]	G_4_3	[1394.697-1428]	Tb_2_3
Standard entropy		Ionic radii, A	
for corresponding		[0.12-0.129]	Rs_1_3
simple oxides,		[0.255-0.267]	Rs_2_3
cal/mol*K		[0.405-0.417]	Rs_3_3
[17.5-17.5324]	So_1_3	(0.417-0.42]	Rs_4_3

Feature	Gradation	Feature	Gradation
[18.4828-18.526]	So_2_3		
[18.5476-18.58]	So_3_3		

2.1.3. COMPUTER LEARNING AND PREDICTION OF CRYSTAL STRUCTURE

The computer learning is carried out for three learning sets in which the compounds from Table 2.1.1.1 were described in terms of the sets of the component properties 2.1.1, 2.1.2 and 2.1.3. The system of concept formation CONFOR [18-20] was used for computer learning and prediction.

The table of predictions of the crystal structure type for the compounds of composition $A_2B_2(XO_4)_3$ (Table 2.1.3.1) results from the comparison of the results of prediction with use of the descriptions in terms of the Features Sets 2.1.1, 2.1.2 and 2.1.3. The following designations are used:

L - langbeinite;
K - $K_2Zn_2(MoO_4)_3$;
- - the crystal structure differing from those listed above;
* - the compound of composition $A_2B_2(XO_4)_3$ does not form.

The physical-chemical systems, which were investigated experimentally, were marked by round brackets. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. The designation "?" corresponds to the indeterminate result of predicring. According to our results the new compounds of the composition $Na_2Mg_2(SO_4)_3$, $K_2Fe_2(SO_4)_3$, $Rb_2B_2(SO_4)_3$ (B = Ca, Fe, Co, Ni, Cu, or Zn), $Cs_2Mn_2(SO_4)_3$, $Cs_2Ni_2(SO_4)_3$, $Tl_2B_2(SO_4)_3$ (B = Mg, Ni, Cu, or Zn), $Na_2B_2(CrO_4)_3$ (B = Mg, Mn, Fe, Co, Ni, Cu, or Zn), $K_2Mg_2(CrO_4)_3$, $Rb_2B_2(CrO_4)_3$ (B = Ca, Fe, Co, Ni, Cu, or Zn), $Cs_2B_2(CrO_4)_3$ (B = Mg, Ca, Mn, Fe, Co, Ni, Cu, or Zn), $Tl_2B_2(CrO_4)_3$ (B = Mg, Ca, Mn, Fe, Co, Ni, Cu, or Zn), $Cs_2Mg_2(WO_4)_3$,

$Tl\,Mg\,(WO_4)_3$, $Rb\,Cd\,(WO_4)_3$, $Cs\,Cd\,(WO_4)_3$, $Tl\,Cd\,(WO_4)_3$ have the crystal structure of langbeinite at normal pressure and room temperature. These compounds hold the promise for searching for new EO materials.

Table 2.1.3.1

Table of Predictions of Crystal Structure Type for Compounds of Composition $A_2B_2(XO_4)_3$

	X = S					X = Cr					X = Mo					X = W				
A / B	Na	K	Rb	Cs	Tl	Na	K	Rb	Cs	Tl	Na	K	Rb	Cs	Tl	Na	K	Rb	Cs	Tl
Mg	L	(L)	(L)	(*)	L	L	L		L	L	K	(K)	(L)	(L)	(L)		(-)	(L)	L	L
Ca	(*)	(L)	L	(L)	(*)			L	L	L	(*)	?	?	?	?	(*)	*	?	?	?
Mn	(*)	(L)	(L)	L	(L)	L		(L)	L	L	K	(-)	(L)	(L)	(L)					
Fe	*	L	L		(L)	L	K	L	L	L	K	K	?	?	?		K			
Co	(*)	(L)	L		(L)	L	K	L	L	L		(K)	(L)	(L)	(-)		K			
Ni	(*)	(L)	L	L	L	L		L	L	L	K	(K)	(L)	(L)	(L)					
Cu	(*)		L	*	L	L	K	L	L	L	K	(K)	?	?	?		K			
Zn	*	(L)	L	*	L	L	K	L	L	L	(-)	(K)	(K)	-	(K)		K			
Sr	(*)	?	?		(*)	*	*	?	?	?	(*)	?	?	?	?	(*)	*	*	*	*
Cd	(*)	(L)	(L)		(L)							K	(-)	(L)	K	(*)		L	L	L
Ba	(*)		(*)	(*)	(*)	*	*				(*)		*	*	*	*	*			
Pb					*	(*)	*	*	*	*	(*)	*	(*)	*	*	(*)	*	(*)	(*)	*

2.2. PREDICTION OF NEW COMPOUNDS WITH COMPOSITION ABX_2O_7

There are many other natural and synthetic members of family of melilite (space group $P\bar{4}2_1m$, Z=2) with general formula $A_1T_2O_7$ (A are

Na^+, Ca^{2+}, Sr^{2+}, Ba^{2+}, Pb^{2+}, Y^{3+}, Ln^{3+} the large ions in octahedral coordination and T are the ions in tetrahedral coordination Be^{2+}, Zn^{2+}, Co^{2+}, Fe^{2+}, Cu^{2+}, Mn^{2+}, Cd^{2+}, B^{3+}, Al^{3+}, Ga^{3+}, Fe^{3+}, Si^{4+}, Ge^{4+}). The oxygen can be substituted partially or completely by ions F^-, OH^-, S^{2-}, N^{3-}. The melilite structure is formed by tetrahedral layers of tetrahedra MgO_4 and diorthogroups Si_2O_7 forming fivemembered rings, that alternate perpendicularly to axis "c", and layers of Ca--polyhedra (Thomson -cubes) [21-26]. The availability of easily deformable atomic structures (octahedra and tetrahedra) in melilites is favourable for EO properties.

The interest in compounds with melilite structure has quickened because stimulated radiation with ions Nd^{3+} was excited for Ba,Mn and Ba, Zn-germanates with this structure [9,24]. The compounds with a melilite structure $Ca_2Mg[Si_2O_7]$ and $Ca_2Zn[Si_2O_7]$ are used as EO filters for picking out radiation with a required wavelength. The dispersion of birefringence in these compounds is characterized by availability of so named wavelength of quasi-isotropy when delta(n)=0 and ellipsoidal optical indicatrix becomes spherical one for monoaxial crystal. In this case the transmission of filter is equal to zero at crossing polarizer and analyzer and, on the contrary, is high along the whole aperture at application of field of displacement that deforms the indicatrix [9].

The composition of melilite varies from akermanite, $Ca_2MgSi_2O_7$, to gehlenite, $Ca_2SiAl_2O_7$. In this work we carried out the prediction of both compounds: similar to the akermanite-melilite structure, $A^{II}_2B^{II}X^{IV}_2O_7$, and analogues of the gehlenite-melilite structure, $A^{II}_2B^{IV}X^{III}_2O_7$.

Previously the efforts of the search for two-dimensional (using ionic

radii A and B) fields of the stability for akermanite-melilite, $A^{II}_2B^{II}X^{IV}_2O_7$, and gehlenite-melilite, $A^{II}_2B^{IV}X^{III}_2O_7$, [21,22] were undertaken. Despite considerable intersection of fields of stability thus found it was assumed that melilites do not form by ions which have more small sizes than Ca^{2+} because of discrepancies of sizes of A-ions and more large polyhedra that contain these ions. The authors of [21,22] mentioned that the stability of melilite structure is determined not only by geometrical factors but also the all set of elements' properties: thermodynamical properties, nature of distribution of ions in structures (ordered or unordered), valency of ions and balance of valent forces on them, nature of the chemical compound and etc. [21].

2.2.1. PREDICTION OF NEW COMPOUNDS OF COMPOSITION $A^{II}_2B^{II}X^{IV}_2O_7$

2.2.1.1. DATA FOR COMPUTER LEARNING

The data for computer learning was extracted from our the cardfile on quaternary inorganic compound properties. On the base of analysis of these data it may be concluded that only compounds $A^{II}_2B^{II}X^{IV}_2O_7$ with X = Si and Ge can crystallize in melilite structure. Therefore this structure at room state and normal pressure was predicted only for silicates and germanates and their analogs in Periodical Table (IV-group): stannates, titanates, zirconates, and hafnates. The table 2.2.1.1.1 contains a learning set.

Table 2.2.1.1.1

Learning Set for Prediction of the Melilite Crystal Structure for Compounds with Composition $A^{II}_2B^{II}X^{IV}_2O_7$

Composition	Crystal type	Space group
Ca2BeSi207	melilite	
Ca2MgSi207	melilite	
Sr2MgSi207	melilite	
Ca2MnSi207	melilite	
Ca2FeSi207	melilite	
Ca2CoSi207	melilite	

Composition	Crystal type	Space group
Ca2ZnSi2O7	melilite	
Ca2CdSi2O7	melilite	
Sr2MnSi2O7	melilite	
Ba2MnSi2O7	melilite	
Pb2MnSi2O7	melilite	
Ba2FeSi2O7	melilite	
Pb2FeSi2O7	melilite	
Sr2CoSi2O7	melilite	
Ba2CoSi2O7	melilite	
Sr2CuSi2O7	melilite	
Sr2ZnSi2O7	melilite	
Ba2ZnSi2O7	melilite	
Pb2ZnSi2O7	melilite	
Sr2CdSi2O7	melilite	
Ba2CdSi2O7	melilite	
Ca2ZnGe2O7	melilite	
Ba2CdGe2O7	melilite	
Ba2MgSi2O7	melilite	
Sr2MnGe2O7	melilite	
Sr2FeSi2O7	melilite	
Ba2CuSi2O7		A2/a, Z=4
Pb2PbSi2O7	barysilite	R3c, Z=18
Pb2PbGe2O7	barysilite	R3c, Z=18
MgO-TiO2	without compound A2BX2O7	
MgO-ZrO2	without compound A2BX2O7	
MgO-HfO2	without compound A2BX2O7	
ZnO-SiO2	without compound A2BX2O7	
ZnO-TiO2	without compound A2BX2O7	
ZnO-ZrO2	without compound A2BX2O7	
FeO-ZrO2	without compound A2BX2O7	

2.2.1.2. SELECTION OF FEATURES

On the basis of physical-chemical grounds two sets of chemical elements features and set of simlpe oxides feature were selected for the description of these systems.

2.2.1.2.1. FEATURE SET 2.2.1.1

The first feature set (feature set 2.2.1.1) includes information about the number of electrons in energy shells of isolated atoms and

Shannon effective ionic radii of elements A (C.N.=8), B (C.N.=4) or X (C.N.=4) in the compound of composition $A_2BX_2O_7$. The grouping of energy shell information corresponds to the number of electrons for each shell. The quasi-continuous properties - the ionic radii - were divided using the special program of discretization [18]. Table 2.2.1.2.1.1 contains the gradations for Feature Set 2.2.1.1.

Table 2.2.1.2.1.1

Gradations for Feature Set 2.2.1.1

Feature	Gradation	Feature	Gradation
	A-element		
3s-shell		5s-shell	
s2	s3_2_1	s0	s5_0_1
3p-shell		s2	s5_2_1
p0	p3_0_1	5p-shell	
p6	p3_6_1	p0	p5_0_1
3d-shell		p6	p5_6_1
d0	d3_0_1	5d-shell	
d5	d3_5_1	d0	d5_0_1
d6	d3_6_1	d10	d5_10_1
d7	d3_7_1	6s-shell	
d10	d3_10_1	s0	s6_0_1
4s-shell		s2	s6_2_1
s0	s4_0_1	6p-shell	
s2	s4_2_1	p0	p6_0_1
4p-shell		p2	p6_2_1
p0	p4_0_1	p6	p6_6_1
p6	p4_6_1	7s-shell	
4d-shell		s0	s7_0_1
d0	d4_0_1	s2	s7_2_1
d10	d4_10_1	Ionic radius, A	
4f-shell		[0.89-0.96]	R1_1
f0	f4_0_1	[1.11-1.14]	R2_1
f6	f4_6_1	[1.25-1.2716]	R3_1
f7	f4_7_1	[1.2822-1.3034]	R3_1
f14	f4_14_1	[1.4094-1.48]	R4_1
	B-element		
2s-shell		4f-shell	
s2	s2_2_2	f0	f4_0_2
2p-shell		f14	f4_14_2
p0	p3_0_2	5s-shell	
p6	p3_6_2	s0	s5_0_2

Feature	Gradation	Feature	Gradation
3s-shell		s2	s5_2_2
s0	s3_0_2	5p-shell	
s2	s3_2_2	p0	p5_0_2
3p-shell		p6	p5_6_2
p0	p3_0_2	5d-shell	
p6	p3_6_2	d0	d5_0_2
3d-shell		d10	d5_10_2
d0	d3_0_2	6s-shell	
d5	d3_5_2	s0	s6_0_2
d6	d3_6_2	s2	s6_2_2
d7	d3_7_2	6p-shell	
d8	d3_8_2	p0	p6_0_2
d10	d3_10_2	p2	p6_2_2
4s-shell		Ionic radius, A	
s0	s4_0_2	[0.27-0.2913]	R1_2
s1	s4_1_2	[0.55-0.5753]	R2_2
s2	s4_2_2	(0.5753-0.5966]	R3_2
4p-shell		(0.5966-0.6179]	R4_2
p0	p4_0_2	[0.6321-0.6534]	R5_2
p6	p4_6_2	(0.6534-0.6747]	R6_2
4d-shell		[0.7599-0.7954]	R7_2
d0	d4_0_2	[0.96-0.98]	R8_2
d10	d4_10_2		
	X-element		
3p-shell		5s-shell	
p2	p3_2_3	s0	s5_0_3
p6	p3_6_3	s2	s5_2_3
3d-shell		5p-shell	
d0	d3_0_3	p0	p5_0_3
d2	d3_2_3	p2	p5_2_3
d10	d3_10_3	p6	p5_6_3
4s-shell		5d-shell	
s0	s4_0_3	d0	d5_0_3
s2	s4_2_3	d2	d5_2_3
4p-shell		d10	d5_10_3
p0	p4_0_3	6s-shell	
p2	p4_2_3	s0	s6_0_3
p6	p4_6_3	s2	s6_2_3
4d-shell		Ionic	
d0	d4_0_3	radius, A	
d2	d4_2_3	[0.26-0.2699]	R1_3
d10	d4_10_3	[0.3821-0.3986]	R2_3

Feature	Gradation	Feature	Gradation
4f-shell		[0.4118-0.4283]	R3_3
f0	f4_0_3	[0.55-0.59]	R4_3
f14	f4_14_3		

2.2.1.2.2. FEATURE SET 2.2.1.2

The second feature set (feature set 2.2.1.2) includes the following information: the first three ionization potentials, the electronegativities by Pauling, the entropies of the individual substances at 298 K, the isobaric thermal capacities at 298 K, the temperatures and the heats of melting and boiling, Debye (characteristic) temperatures, the energies of the crystal lattice, the ionic radii by Shannon, the ratio of the atomic number to the average atomic mass for atoms of elements A, B and X. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.2.1.2.2.1 contains the gradations for Feature Set 2.2.1.2.

Table 2.2.1.2.2.1

Gradations for Feature Set 2.1.2.2

Feature	Gradation	Feature	Gradation
	A-element		
First ionization		Boiling point, K	
potential, eV		[630-1238.319]	Tb_1_1
[5.21166-5.337139]	I1_1_1	[1316.945-1415.228]	Tb_2_1
[5.588098-5.79723]	I1_2_1	[1593-1880]	Tb_3_1
[6.048188-6.254]	I1_3_1	[1943-2063.893]	Tb_4_1
[7.30298-7.512112]	I1_4_1	[2103.206-2350]	Tb_5_1
[7.595765-7.763071]	I1_5_1	[3086.031-3230]	Tb_6_1
[7.846724-8.014029]	I1_6_1	Heat of melting,	
[8.9939-10.4376]	I1_7_1	kJ/mol	
Second ionization		[2.295-5.046776]	Hm_1_1
potential, eV		[6.234-7.203863]	Hm_2_1
[10.004-10.2428]	I2_1_1	(7.203863-7.473498]	Hm_3_1
[10.8796-11.24]	I2_2_1	[7.95-8.462163]	Hm_4_1
[11.6756-12.18]	I2_3_1	(8.462163-11.09502]	Hm_5_1
[14.9392-15.64]	I2_4_1	[12.05-16.318]	Hm_6_1
[16.0536-17.084]	I2_5_1	Heat of boiling,	
[17.8048-18.76]	I2_6_1	kJ/mol	
Third ionization		[59.229-122.3451]	Hb_1_1
potential, eV		[136.4134-148.1369]	Hb_2_1
[23.4-31.63988]	I3_1_1	(148.1369-157.737]	Hb_3_1

Feature	Gradation	Feature	Gradation
(31.63988-34.2]	I3_2_1	[162.2052-166.8946]	Hb_4_1
[35.10446-37.47]	I3_3_1	(166.8946-173.9288]	Hb_5_1
[39.06398-41.04374]	I3_4_1	(173.9288-226.773]	Hb_6_1
[42.03362-44.01338]	I3_5_1	[342.7479-375.723]	Hb_7_1
[49.95266-51.93242]	I3_6_1	Energy of the crystal lattice, -6 E*10 J/kg*mol	
[78.65918-80.144]	I3_7_1	[116-139.72]	E_1_1
Electronegativity		[145.2-156.16]	E_2_1
[0.9-0.927]	X_1_1	(156.16-169.86]	E_3_1
[0.9809999-1.026]	X_2_1	(169.86-183.56]	E_4_1
[1.1-1.224]	X_3_1	[189.04-286]	E_5_1
[1.5-1.62]	X_4_1	[364.7-430]	E_6_1
[1.7-1.9]	X_5_1	Debye temperature, K	
Entropies of individual substances at 298 K kJ/kg*mol*K		[75-106.16]	Td_1_1
[27.154-28.3723]	S_1_1	[121.04-147]	Td_2_1
[30.041-33.6516]	S_2_1	[190-228.92]	Td_3_1
[40.9614-42.5858]	S_3_1	[295.88-314.48]	Td_4_1
[51.756-56.7993]	S_4_1	[396.32-414.92]	Td_5_1
[61.6725-63.2969]	S_5_1	[445-467]	Td_6_1
[66.5457-79.898]	S_6_1	Ratio of the atomic number to the average atomic mass	
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		[0.39-0.403	NM_1_1
[24.811-25.1208]	Cp_1_1	[0.407-0.412]	NM_2_1
[25.372-25.531]	Cp_2_1	[0.428-0.432]	NM_3_1
[25.849-26.024]	Cp_3_1	[0.458-0.462]	NM_4_1
[26.2676-26.5168]	Cp_4_1	[0.468-0.472]	NM_5_1
[26.7076-26.8666]	Cp_5_1	[0.488-0.492]	NM_6_1
[27.983-29.288]	Cp_6_1	[0.498-0.5]	NM_7_1
Melting point, K		Ionic radius, A	
[234.29-636.942]	Tm_1_1	[0.89-0.96]	Rs_1_1
[661.17-721.74]	Tm_2_1	[1.11-1.14]	Rs_2_1
[891.336-951.906]	Tm_3_1	[1.25-1.2716]	Rs_3_1
[976.134-1024.59]	Tm_4_1	[1.2822-1.3034]	Rs_4_1
(1024.59-1073.046]	Tm_5_1	[1.4094-1.48]	Rs_5_1
[1097-1345]	Tm_6_1		
[1558-1812]	Tm_7_1		

Feature	Gradation	Feature	Gradation
	B-element		
First ionization potential, eV		Heat of melting, kJ/mol	
[7.4167-7.476028]	I1_1_2	[2.295-5.123366]	Hm_1_2
[7.594684-7.772668]	I1_2_2	[6.046635-6.508269]	Hm_2_2
[7.81222-7.891324]	I1_3_2	[6.969903-7.546947]	Hm_3_2
(7.891324-8.336]	I1_4_2	[8.239398-8.816442]	Hm_4_2
[8.939452-9.038332]	I1_5_2	[11.81707-12.85574]	Hm_5_2
[9.275644-9.374524]	I1_6_2	(12.85574-13.20197]	Hm_6_2
(9.374524-10.4376]	I1_7_2	[13.43279-14.00983]	Hm_7_2
Second ionization potential, eV		[16.08718-19.665]	Hm_8_2
		Heat of boiling, kJ/mol	
[15.033-15.1908]	I2_1_2	[59.229-107.8633]	Hb_1_2
[15.5064-15.7694]	I2_2_2	(107.8633-121.6705]	Hb_2_2
[16.085-16.2954]	I2_3_2	[138.2392-149.2849]	Hb_3_2
[16.8214-17.1896]	I2_4_2	[171.3764-185.1836]	Hb_4_2
[17.8208-18.0838]	I2_5_2	[223.8438-234.8896]	Hb_5_2
(18.0838-18.76]	I2_6_2	[295.6412-309.4484]	Hb_6_2
[19.43-20.293]	I2_7_2	(309.4484-320.4942]	Hb_7_2
Third ionization potential, eV		[342.5857-356.3929]	Hb_8_2
[29-31.8825]	I3_1_2	[367.4387-510.448]	Hb_9_2
(31.8825-33.115]	I3_2_2	Energy of the crystal lattice, -6 E*10 J/kg*mol	
(33.115-36.8125]	I3_3_2		
(36.8125-42.975]	I3_4_2		
[77.485-83.6475]	I3_5_2		
[150.2025-153.9]	I3_6_2	[116-125.42]	E_1_2
Electronegativity		(125.42-137.98]	E_2_2
[1.2-1.221]	X_1_2	[144.26-156.82]	E_3_2
[1.487-1.515]	X_2_2	[188.22-200.78]	E_4_2
[1.585-1.62]	X_3_2	[282.42-294.98]	E_5_2
[1.69-1.718]	X_4_2	[313.82-329.52]	E_6_2
[1.788-1.816]	X_5_2	[335.8-348.36]	E_7_2
[1.886-2.2]	X_6_2	[390-414.3]	E_8_2
Entropies of individual substances at 298 K kJ/kg*mol*K		[420.58-510]	E_9_2
		Debye temperature, K	
		[75-126.95]	Td_1_2
[9.498-11.24598]	S_1_2	[169.55-233]	Td_2_2
[26.39514-28.72578]	S_2_2	[275-329.3]	Td_3_2
(28.72578-32.22174]	S_3_2	(329.3-371.9]	Td_4_2
(32.22174-37.656]	S_4_2	[393.2-435.8]	Td_5_2
[40.37898-43.29228]	S_5_2	(435.8-457.1]	Td_6_2

Feature	Gradation	Feature	Gradation
[50.2842-53.1975]	S_6_2	(457.1-489.05]	Td_7_2
[66.01602-79.898]	S_7_2	[1128.05-1160]	Td_8_2
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		Ratio of the atomic number to the average atomic mass	
[16.443-16.743]	Cp_1_2		
[24.143-24.643]	Cp_2_2	[0.4-0.4027]	NM_1_2
(24.643-24.843]	Cp_3_2	[0.4279-0.4324]	NM_2_2
(24.843-24.943]	Cp_4_2	[0.4378-0.4423]	NM_3_2
(24.943-25.643]	Cp_5_2	[0.4585-0.4621]	NM_4_2
[25.843-26.343]	Cp_6_2	[0.4675-0.472]	NM_5_2
(26.343-27.983]	Cp_7_2	[0.48-0.49]	NM_6_2
Melting point, K		Ionic radius, A	
[234.29-630.54]	Tm_1_2	[0.27-0.2913]	Rs_1_2
[679.26-727.98]	Tm_2_2	[0.55-0.5753]	Rs_2_2
[898.5-959.4]	Tm_3_2	(0.5753-0.5966]	Rs_3_2
[1324.8-1385.7]	Tm_4_2	(0.5966-0.6179]	Rs_4_2
[1531.86-1592.76]	Tm_5_2	[0.6321-0.6534]	Rs_5_2
[1728-1799.82]	Tm_6_2	(0.6534-0.6747]	Rs_6_2
(1799.82-2045]	Tm_7_2	[0.7599-0.7954]	Rs_7_2
Boiling point, K		[0.96-0.98]	Rs_8_2
[630-1105.36]	Tb_1_2		
[1149.167-1236.781]	Tb_2_2		
[1324.396-1412.01]	Tb_3_2		
[1981.5-2069.115]	Tb_4_2		
[2288.149-2397.667]	Tb_5_2		
[2704.316-2791.93]	Tb_6_2		
(2791.93-2937]	Tb_7_2		
[3098.579-3208.096]	Tb_8_2		
(3208.096-4100]	Tb_9_2		
	X-element		
First ionization potential, eV		Boiling point, K	
		[2890-3173.1]	Tb_1_3
[6.634-6.679531]	I1_1_3	[3491.7-3562.5]	Tb_2_3
[6.770593-7.344]	I1_2_3	(3562.5-3651]	Tb_3_3
[7.863337-7.939222]	I1_3_3	[4571.4-4659.9]	Tb_4_3
[8.121346-8.1517]	I1_4_3	[4836.9-4890]	Tb_5_3
Second ionization potential, eV		Heat of melting, kJ/mol	
[13.13-13.22648]	I2_1_3	[4.64735-7.2013]	Hm_1_3
[13.48376-13.64456]	I2_2_3	[14.15767-15.788]	Hm_2_3
[14.632-14.99528]	I2_3_3	[20.13558-21.49419]	Hm_3_3

Feature	Gradation	Feature	Gradation
[15.89576-16.0244]	I2_4_3	[31.27623-31.81968]	Hm_4_3
[16.28168-16.346]	I2_5_3	Heat of boiling,	
Third ionization		kJ/mol	
potential, eV		[296.102-385.8269]	Hb_1_3
[23.1-23.544]	I3_1_3	[389.6042-397.1587]	Hb_2_3
[27.318-27.762]	I3_2_3	[408.4904-416.045]	Hb_3_3
[30.5-33.756]	I3_3_3	[555.8036-569.024]	Hb_4_3
[33.978-34.2]	I3_4_3	Energy of the	
Electronegativity		crystal lattice,	
[1.3-1.321]	X_1_3	-6	
[1.391-1.419]	X_2_3	E*10 J/kg*mol	
[1.489-1.517]	X_3_3	[302-336.165]	E_1_3
[1.783-1.818]	X_4_3	[366.825-377.045]	E_2_3
[1.986-2]	X_5_3	[463.915-476.69]	E_3_3
Entropies of		[578.89-584]	E_4_3
individual		Debye	
substances at 298 K		temperature, K	
kJ/kg*mol*K		[190-272.3]	Td_1_3
[18.828-19.56981]	S_1_3	[305.1-321.5]	Td_2_3
[29.95515-30.94423]	S_2_3	[362.5-378.9]	Td_3_3
(30.94423-31.68604]	S_3_3	[419.9-440.4]	Td_4_3
[38.6096-39.59868]	S_4_3	[661.8-670]	Td_5_3
[43.06046-44.141]	S_5_3	Ratio of the	
Isobaric thermal		atomic number	
capacity at 298 K,		to the average	
kJ/kg*mol*K		atomic mass	
[20.041-20.21173]	Cp_1_3	[0.4-0.42]	NM_1_3
[23.28487-23.51251]	Cp_2_3	[0.437-0.442]	NM_2_3
[24.99217-25.50436]	Cp_3_3	[0.458-0.462]	NM_3_3
[25.61818-25.773]	Cp_4_3	[0.498-0.5]	NM_4_3
Melting point, K		Ionic radius, A	
[505-1249.088]	Tm_1_3	[0.26-0.2699]	Rs_1_3
[1661.76-1713.344]	Tm_2_3	[0.3821-0.3986]	Rs_2_3
[1919.68-1971.264]	Tm_3_3	[0.4118-0.4283]	Rs_3_3
[2100.224-2164.704]	Tm_4_3	[0.55-0.59]	Rs_4_3
[2474.208-2500]	Tm_5_3		

2.2.1.2.3. FEATURE SET 2.2.1.3

The third set of properties of simple oxides (feature set 2.2.1.3) includes the following information of simple oxides AO, BO and XO :

melting and boiling (only for AO and BO) points, standard enthalpy of formation, standard isobaric thermal capacities, standard entropies, standard Gibbs energy, effective ionic radii of correspoding cations by Shannon. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.2.1.2.3.1 contains the gradations for Feature Set 2.2.1.3.

Table 2.2.1.2.3.1

Gradations for Feature Set 2.2.1.3
(Properties of Simple Oxides)

Feature	Gradation	Feature	Gradation
	AO		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
		[8.89-8.9812]	Cp_1_1
[21.704-57.1]	H_1_1	[9.5892-9.7108]	Cp_2_1
[60.99111-65.98006]	H_2_1	[10.0148-10.1364]	Cp_3_1
[81.9447-92.4]	H_3_1	[10.43-10.8356]	Cp_4_1
[123-133.8298]	H_4_1	[10.8964-11.018]	Cp_5_1
[139.8165-142.8099]	H_5_1	[11.1396-11.5]	Cp_6_1
(142.8099-145.8033]	H_6_1	[11.8388-13.2]	Cp_7_1
[149.7944-151.79]	H_7_1	Melting point of simple oxides, K	
Standard Gibbs energy for simple oxides, kcal/mol		[1159-1216.42]	Tm_1_1
		[1599.22-1694.92]	Tm_2_1
		[2090-2288.26]	Tm_3_1
[14.015-47.95956]	G_1_1	(2288.26-2345.68]	Tm_4_1
[51.411-60.86232]	G_2_1	[2805.04-2977.3]	Tm_5_1
[74.7576-86.837]	G_3_1	[3015.58-3073]	Tm_6_1
[116.738-126.3686]	G_4_1	Boiling point of simple oxides, K	
[132.3238-135.3013]	G_5_1		
(135.3013-138.2789]	G_6_1	[1746-1809.81]	Tb_1_1
[142.249-144.234]	G_7_1	[3086.01-3171.09]	Tb_2_1
Standard entropy for corresponding simple oxides, cal/mol*K		[3809.19-3873]	Tb_3_1
		Ionic radii, A	
		[0.89-0.96]	Rs_1_1
		[1.101.14]	Rs_2_1
[6.47-6.7919]	So_1_1	[1.2504-1.2716]	Rs_3_1
[10.2255-10.6547]	So_2_1	[1.2822-1.3034]	Rs_4_1
[12.6-13.4445]	So_3_1	[1.4094-1.48]	Rs_5_1
[14.3029-14.8394]	So_4_1		
[16.127-16.6635]	So_5_1		
[16.8-20]	So_6_1		

Feature	Gradation	Feature	Gradation
	BO		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
[21.704-41.9264]	H_1_2	[6.11-7.5]	Cp_1_2
[50.4768-54.752]	H_2_2	[8.7333-9.0878]	Cp_2_2
(54.752-62.2336]	H_3_2	[9.5132-9.7968]	Cp_3_2
(62.2336-65.44]	H_4_2	[9.9386-10.293]	Cp_4_2
[82.5408-86.816]	H_5_2	(10.2931-10.7185]	Cp_5_2
[91.09121-95.36641]	H_6_2	[10.8603-11.1439]	Cp_6_2
[142.3936-144.5312]	H_7_2	[11.8529-12.1365]	Cp_7_2
(144.5312-145.6]	H_8_2	[12.9873-13.2]	Cp_8_2
Standard Gibbs energy for simple oxides, kcal/mol		Melting point of simple oxides, K	
		[780-1216.42]	Tm_1_2
		[1484.38-1560.94]	Tm_2_2
		[1599.22-1694.92]	Tm_3_2
[14.015-34.1494]	G_1_2	[2039.44-2154.28]	Tm_4_2
[42.7638-48.1478]	G_2_2	[2192.56-2288.26]	Tm_5_2
[50.3014-57.839]	G_3_2	[2785.9-2862.46]	Tm_6_2
(57.839-61.0694]	G_4_2	[3015.58-3073]	Tm_7_2
[73.991-79.375]	G_5_2	Boiling point of simple oxides, K	
[83.6822-89.0662]	G_6_2		
[134.2918-137.5222]	G_7_2	[1746-2263]	Tb_1_2
(137.5222-138.599]	G_8_2	[3800.97-3927.82]	Tb_2_2
Standard entropy for corresponding simple oxides, cal/mol*K		[4232.26-4283]	Tb_3_2
		Ionic radii, A	
		[0.27-0.2913]	Rs_1_2
		[0.55-0.5753]	Rs_2_2
[3.29-3.6839]	So_1_2	(0.5753-0.5966]	Rs_3_2
[6.3099-6.8351]	So_2_2	[0.5966-0.6179]	Rs_4_2
[9.08-10.3802]	So_3_2	[0.6321-0.6534]	Rs_5_2
(10.3802-10.7741]	So_4_2	(0.6534-0.6747]	Rs_6_2
[12.3497-13.5]	So_5_2	[0.7599-0.7954]	Rs_7_2
[14.1879-14.5818]	So_6_2	[0.9-0.98]	Rs_8_2
(14.5818-14.9757]	So_7_2		
[16.0261-16.8]	So_8_2		

Feature	Gradation	Feature	Gradation
	XO_2		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
[138.66-142.5132]	H_1_3	[10.62-10.7334]	Cp_1_3
[214.4396-220.8616]	H_2_3	[11.943-12.6]	Cp_2_3
[223.4304-228.568]	H_3_3	[13.077-13.2282]	Cp_3_3
[259.3936-267.1]	H_4_3	[13.3794-13.5306]	Cp_4_3
Standard Gibbs energy for simple oxides, kcal/mol		[14.2866-14.4]	Cp_5_3
		Melting point of simple oxides, K	
[124.253-128.5286]	G_1_3	[1389-1439.82]	Tm_1_3
[203.3213-208.4795]	G_2_3	[1846.38-1931.08]	Tm_2_3
[211.0585-216.2166]	G_3_3	[2100.48-2273]	Tm_3_3
[247.1654-253.613]	G_4_3	[2930.54-3015.24]	Tm_4_3
		[3049.12-3083]	Tm_5_3
Standard entropy for corresponding simple oxides, cal/mol*K		Ionic radii, A	
		[0.26-0.2699]	Rs_1_3
		[0.3821-0.3986]	Rs_2_3
		[0.4118-0.4283]	Rs_3_3
		[0.55-0.59]	Rs_4_3
[9.49-9.6307]	So_1_3		
[9.9121-10.0997]	So_2_3		
[11.9757-12.5]	So_3_3		
[14.0393-14.18]	So_4_3		

2.2.1.3. COMPUTER LEARNING AND PREDICTION OF CRYSTAL STRUCTURE

The computer learning is carried out for three learning sets in which the compounds from Table 2.2.1.1.1 were described in terms of the sets of the component properties 2.2.1.1, 2.2.1.2 and 2.2.1.3. The system of concept formation CONFOR [18-20] was used for computer learning and prediction.

The tables of predictions of the crystal structure type for the compounds of composition $A_2^{II}B_2^{II}X_2^{IV}O_7$ (Tables 2.2.1.3.1-2.2.1.3.6) result from the comparison of the results of prediction with use of the descriptions in terms of the Features Sets 2.2.1.1, 2.2.1.2 and

2.2.1.3. The following designations are used:

M - melilite;
- - the crystal structure differing from those listed above;
* - the compound of composition $A_2BX_2O_7$ does not form.

The physical-chemical systems, which were investigated experimentally, were marked by round brackets. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. The designation "?" corresponds to the indeterminate result of predicting. According to our results the new compounds of the composition $A_2BSi_2O_7$ (A = Ca^{2+}, Sr^{2+}, Sm^{2+}, or Eu^{2+}; B = Be^{2+}, Mg^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Pd^{2+}, Cd^{2+}, Hg^{2+}, or Pb^{2+}), $Ba_2NiSi_2O_7$, $Ba_2PdSi_2O_7$, $A_2BSi_2O_7$ (A = Yb^{2+}, Hg^{2+}, or Pb^{2+}; B = Mn^{2+}, Fe^{2+}, Zn^{2+}, or Cd^{2+}), $Ra_2BSi_2O_7$ (B = Mg^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Pd^{2+}, Cd^{2+}, Hg^{2+}, or Pb^{2+}), $A_2BX_2O_7$ (A = Ca^{2+} or Sr^{2+}; B = Be^{2+}, Mg^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, Pd^{2+}, Cd^{2+}, Hg^{2+}, or Pb^{2+}; X = Ge^{4+} or Ti^{4+}), $A_2BX_2O_7$ (A = Ba^{2+}, Sm^{2+}, Eu^{2+}, Hg^{2+}, or Ra^{2+}; B = Mn^{2+}, Ni^{2+}, or Cd^{2+}; X = Ge^{4+}, Sn^{4+}, Ti^{4+}, Zr^{4+}, or Hf^{4+}), $A_2PdX_2O_7$ (A = Sm^{2+}, Eu^{2+}, or Ra^{2+}; X = Ge^{4+}, Sn^{4+}, Ti^{4+}, Zr^{4+}, or Hf^{4+}), $Ra_2HgX_2O_7$ (X = Ge^{4+}, Sn^{4+}, Ti^{4+}, Zr^{4+}, or Hf^{4+}) have the crystal structure of melilite at normal pressure and room temperature. These compounds hold the promise for searching for new EO materials.

Table 2.2.1.3.1

Table of Predictions of Crystal Structure Type

for Compounds of Composition $A_2^{II} B_2^{II} Si_2^{IV} O_7$

A / B	Mg	Ca	Mn	Fe	Co	Zn	Sr	Cd	Ba	Sm	Eu	Yb	Hg	Pb	Ra
Be	?	(M)	?	?	?	?	M	?		M	M	-	-	-	
Mg	?	(M)	?	?	?	?	(M)	?	(M)	M	M	-	-	-	M
Mn	?	(M)	?	?	?	?	(M)	?	(M)	M	M	M	M	(M)	M
Fe	?	(M)	?	?	?	?	(M)	?	(M)	M	M	M	M	(M)	M
Co	?	(M)	?	?	?	?	(M)	?	(M)	M	M	-	-	-	M
Ni	?	M	?	?	?	?	M	?	M	M	M	?	?	?	M
Cu	?	M	?	?	?	?	(M)	?	(-)	M	M	-	-	-	M
Zn	?	(M)	?	?	?	(*)	(M)	?	(M)	M	M	M	M	(M)	M
Pd	?	M	?	?	?	?	M	?	M	M	M	?	?	?	M
Cd	?	(M)	?	?	?	?	(M)		(M)	M	M	M	M	M	M
Hg	?	M	?	?	?	?	M	?		M	M	-		-	M
Pb	?	M	?	?	?	?	M	?	-	M	M	-	-	(-)	M

Table 2.2.1.3.2

Table of Predictions of Crystal Structure Type

for Compounds of Composition $A_2^{II} B_2^{II} Ge^{IV} O_7$

A / B	Mg	Ca	Mn	Fe	Co	Zn	Sr	Cd	Ba	Sm	Eu	Yb	Hg	Pb	Ra
Be	*	M	*	*	*	*	M	?	-	?	?	-	-	-	-
Mg		M	*	*	*	*	M	?	-	?	?	-	-	-	?
Mn	?	M	?	?	?	?	M	?	M	M	M	?	M	?	M
Fe	*	M	*		*	*	M	?	-	?	?	-	-	-	?
Co	*	M	*	*		*	M	?	-	?	?	-	-	-	?
Ni	?	M	?	?	?	?	M	?	M	M	M	?	M	?	M
Cu	*	M	*	*	*	*	M	?	-	?	?	-	-	-	?
Zn	*	(M)	*	*	*		M	?	-	?	?	-	-	-	?
Pd	*	M		*	*	*	M	?	?	M	M	?	?	-	M
Cd	?	M	?	?	?	?	M		(M)	M	M	M	M	M	M
Hg	*	M	*	*	*	*	M	?		?	?	-		-	M
Pb	*	M	*	*	*	*	M	-	-	?	?	-	-	(-)	?

Table 2.2.1.3.3

Table of Predictions of Crystal Structure Type

for Compounds of Composition $A_2^{II}B_2^{II}Sn^{IV}O_7$

A / B	Mg	Ca	Mn	Fe	Co	Zn	Sr	Cd	Ba	Sm	Eu	Yb	Hg	Pb	Ra
Be	*		*	*	*	*		*	–	?	?	–	–	–	–
Mg			*	*	*	*	M	*	–	?	?	–	–	–	?
Mn	?	M		?	?	?	M	?	M	M	M	?	M	?	M
Fe	*	M	*		*	*	M	?	–	?	?	–	–	–	?
Co	*	M	*	*		*	M	?	–	?	?	–	–	–	?
Ni	?	M	?	?	?	?	M	?	M	M	M	?	M	?	M
Cu	*	M	*	*	*	*	M	?	–	?	?	–	–	–	?
Zn	*	M	*	*	*		M	?	–	?	?	–	–	–	?
Pd	*	M	*	*	*	*	M	?	?	M	M	?	?	–	M
Cd	?	M	?	?	?	?	M		M	M	M	?	M	?	M
Hg	*	M	*	*	*	*	M			?	?	–		–	M
Pb	*	M	*	*	*	*	M	–	–	?	?	–	–		–

Table 2.2.1.3.4

Table of Predictions of Crystal Structure Type

for Compounds of Composition $A_2^{II} B_2^{II} Ti^{IV} O_7$

A / B	Mg	Ca	Mn	Fe	Co	Zn	Sr	Cd	Ba	Sm	Eu	Yb	Hg	Pb	Ra
Be	*	M	*	*	*	*	M	?	-	?	?	-	-	-	-
Mg	(*)	M	*	*	*	*	M	?	-	?	?	-	-	-	?
Mn	?	M	?	?	?	?	M	?	M	M	M	?	M	?	M
Fe	*	M	*		*	*	M	?	-	?	?	-	-	-	?
Co	*	M	*	*		*	M	?	-	?	?	-	-	-	?
Ni	?	M	?	?	?	?	M	?	M	M	M	?	M	?	M
Cu	*	M	*	*	*	*	M	?	-	?	?	-	-	-	?
Zn	*	M	*	*	*		M	?	-	?	?	-	-	-	?
Pd	*	M	*	*	*	*	M	?	?	M	M	?	?	-	M
Cd	?	M	?	?	?	?	M		M	M	M	?	M	?	M
Hg	*	M	*	*	*	*	M	?		?	?	-		-	M
Pb	*	M	*	*	*	*	M	-	-	?	?	-	-		-

Table 2.2.1.3.5

Table of Predictions of Crystal Structure Type

for Compounds of Composition $A_2^{II}B_2^{II}Zr_2^{IV}O_7$

A / B	Mg	Ca	Mn	Fe	Co	Zn	Sr	Cd	Ba	Sm	Eu	Yb	Hg	Pb	Ra
Be	*		*	*	*	*	M	*	-	?	?	-	-	-	-
Mg	(*)		*	*	*	*	M	*	-	?	?	-	-	-	?
Mn	?	M		?	?	?	M	?	M	M	M	?	M	?	M
Fe	*	M	*	(*)	*	*	M	?	-	?	?	-	-	-	?
Co	*	M	*	*		*	M	?	-	?	?	-	-	-	?
Ni	?	M	?	?	?	?	M	?	M	M	M	?	M	?	M
Cu	*	M	*	*	*	*	M	?	-	?	?	-	-	-	?
Zn	*	M	*	*	*	(*)	M	?	-	?	?	-	-	-	?
Pd	*	M	*	*	*	*	M	?	?	M	M	?	?	-	M
Cd	?	M	?	?	?	?	M		M	M	M	?	M	?	M
Hg	*	M	*	*	*	*	M	?		?	?	-		-	M
Pb	*	M	*	*	*	*	M	-	-	?	?	-	-		-

Table 2.2.1.3.6

Table of Predictions of Crystal Structure Type
for Compounds of Composition $A_2^{II}B_2^{II}Hf_2^{IV}O_7$

A / B	Mg	Ca	Mn	Fe	Co	Zn	Sr	Cd	Ba	Sm	Eu	Yb	Hg	Pb	Ra
Be	*		*	*	*	*		*	-	?	?	-	-	-	-
Mg	(*)		*	*	*	*	M	*	-	?	?	-	-	-	?
Mn	?	M		?	?	?	M	?	M	M	M	?	M	?	M
Fe	*	M	*		*	*	M	?	-	?	?	-	-	-	?
Co	*	M	*	*		*	M	?	-	?	?	-	-	-	?
Ni	?	M	?	?	?	?	M	?	M	M	M	?	M	?	M
Cu	*	M	*	*	*	*	M	?	-	?	?	-	-	-	?
Zn	*	M	*	*	*		M	?	-	?	?	-	-	-	?
Pd	*	M	*	*	*	*	M	?	?	M	M	?	?	-	M
Cd	?	M	?	?	?	?	M		M	M	M	?	M	?	M
Hg	*	M	*	*	*	*	M	?		?	?	-		-	M
Pb	*	M	*	*	*	*	M	-	-	?	?	-	-		-

2.2.2. PREDICTION OF NEW COMPOUNDS OF COMPOSITION $A_2^{II}X_2^{IV}B_2^{III}O_7$

2.2.2.1. DATA FOR COMPUTER LEARNING

The data for computer learning was extracted from our the cardfile on quaternary inorganic compound properties. On the base of analysis of these data it may be concluded that only compounds $A_2^{II}X_2^{IV}B_2^{III}O_7$ with X = Si and Ge can crystallize in melilite structure. Therefore this structure at room state and normal pressure was predicted only for

silicates and germanates and their analogs in Periodical Table (IV-group): stannates, titanates, zirconates, and hafnates. The table 2.2.2.1.1 contains a learning set.

Table 2.2.2.1.1

Learning Set for Prediction of the Melilite Crystal Structure for Compounds with Composition $A_2^{II} X^{IV} B_2^{III} O_7$

Composition	Crystal type	Space group
Be2SiY207	melilite	
Be2SiNd207	melilite	
Be2SiSm207	melilite	
Be2SiEu207	melilite	
Be2SiGd207	melilite	
Be2SiTb207	melilite	
Be2SiDy207	melilite	
Be2SiHo207	melilite	
Be2SiEr207	melilite	
Be2SiTm207	melilite	
Be2SiYb207	melilite	
Be2SiLu207	melilite	
Be2GeY207	melilite	
Be2GeLa207	melilite	
Be2GePr207	melilite	
Be2GeNd207	melilite	
Be2GeSm207	melilite	
Be2GeEu207	melilite	
Be2GeGd207	melilite	
Be2GeTb207	melilite	
Be2GeDy207	melilite	
Be2GeHo207	melilite	
Be2GeEr207	melilite	
Be2GeTm207	melilite	
Be2GeYb207	melilite	
Be2GeLu207	melilite	
Ca2SiB207	melilite	
Ca2SiAl207	melilite	
Sr2SiAl207	melilite	
Ca2GeAl207	melilite	
Sr2GeAl207	melilite	
Ca2SiGa207	melilite	
Ca2GeGa207	melilite	
Sr2GeFe207	melilite	
Ba2GeFe207	melilite	

Composition	Crystal type	Space group
Sr2GeLa2O7	melilite	
Ba2GeGa2O7	melilite	
Sr2GeGa2O7	melilite	
Mg2SnLa2O7		cubic, Z=3
Mg2SnPr2O7		orthorhombic, Z=2
Mg2SnNd2O7		orthorhombic, Z=2
Ca2SnLa2O7		orthorhombic, Z=2
Ca2SnNd2O7		orthorhombic, Z=2
Zn2SnLa2O7		orthorhombic, Z=2
MgO-Y2O3-ZrO2	without compound A2XB2O7	
MgO-Y2O3-HfO2	without compound A2XB2O7	
MgO-Gd2O3-ZrO2	without compound A2XB2O7	
CaO-Y2O3-ZrO2	without compound A2XB2O7	
CaO-Y2O3-HfO2	without compound A2XB2O7	
CaO-Gd2O3-ZrO2	without compound A2XB2O7	
BaO-Ga2O3-SiO2	without compound A2XB2O7	
BaO-Al2O3-GeO2	without compound A2XB2O7	
CaO-Fe2O3-GeO2	without compound A2XB2O7	

2.2.2.2. SELECTION OF FEATURES

On the basis of physical-chemical grounds two sets of chemical elements features and set of simlpe oxides feature were selected for the description of these systems.

2.2.2.2.1. FEATURE SET 2.2.2.1

The first feature set (feature set 2.2.2.1) includes information about the number of electrons in energy shells of isolated atoms and Bokii and Belov effective ionic radii of elements A, B or X in the compound of composition $A_2XB_2O_7$. The grouping of energy shell information corresponds to the number of electrons for each shell. The quasi-continuous properties - the ionic radii - were divided using the special program of discretization [18]. Table 2.2.2.2.1.1 contains the gradations for Feature Set 2.2.2.1. The use of Bokii and Belov effective ionic radii of elements was caused by the vagueness of C.N. for A^{2+} and B^{3+} in these compounds because both A^{2+} and B^{3+} can have C.N.=8 or C.N.=4. It is impossible to indicate how many ions have one or other coordination. Therefore average ionic radii by Bokii and Be-

lov were chosen.

Table 2.2.2.2.1.1

Gradations for Feature Set 2.2.2.1

Feature	Gradation	Feature	Gradation
	A-element		
2s-shell		5s-shell	
s2	s2_2_1	s0	s5_0_1
3s-shell		s2	s5_2_1
s0	s3_0_1	5p-shell	
s2	s3_2_1	p0	p5_0_1
3p-shell		p2	p5_2_1
p0	p3_0_1	p6	p5_6_1
p6	p3_6_1	5d-shell	
3d-shell		d0	d5_0_1
d0	d3_0_1	d10	d5_10_1
d2	d3_2_1	6s-shell	
d3	d3_3_1	s0	s6_0_1
d5	d3_5_1	s2	s6_2_1
d6	d3_6_1	6p-shell	
d7	d3_7_1	p0	p6_0_1
d8	d3_8_1	p2	p6_2_1
d10	d3_10_1	p6	p6_6_1
4s-shell		7s-shell	
s0	s4_0_1	s0	s7_0_1
s1	s4_1_1	s2	s7_2_1
s2	s4_2_1	Ionic radius, A	
4p-shell		[0.34-0.3712]	R1_1
p0	p4_0_1	[0.65-0.78]	R2_1
p2	p4_2_1	[0.8-0.91]	R3_1
p6	p4_6_1	[0.99-1.068]	R3_1
4d-shell		[1.12-1.26]	R4_1
d0	d4_0_1	[1.3488-1.44]	R5_1
d10	d4_10_1		
4f-shell			
f0	f4_0_1		
f14	f4_14_1		
	B-element		
3p-shell		5s-shell	
p0	p3_0_2	s0	s5_0_2
p1	p3_1_2	s1	s5_1_2
p6	p3_6_2	s2	s5_2_2
3d-shell		5p-shell	
d0	d3_0_2	p0	p5_0_2

Feature	Gradation	Feature	Gradation
d1	d3_1_2	p1	p5_1_2
d2	d3_2_2	p3	p5_3_2
d3	d3_3_2	p6	p5_6_2
d4	d3_4_2	5d-shell	
d5	d3_5_2	d0	d5_0_2
d6	d3_6_2	d1	d5_1_2
d7	d3_7_2	d10	d5_10_2
d10	d3_10_2	6s-shell	
4s-shell		s0	s6_0_2
s0	s4_0_2	s2	s6_2_2
s1	s4_1_2	6p-shell	
s2	s4_2_2	p0	p6_0_2
4p-shell		p6	p6_6_2
p0	p4_0_2	6d-shell	
p1	p4_1_2	d0	d6_0_2
p3	p4_3_2	d1	d6_1_2
p6	p4_6_2	7s-shell	
4d-shell		s0	s7_0_2
d0	d4_0_2	s2	s7_2_2
d1	d4_1_2	Ionic radius, A	
d8	d4_8_2	[0.2-0.2252]	R1_1
d10	d4_10_2	[0.5612-0.64]	R1_1
4f-shell		[0.6536-0.69]	R2_1
f0	f4_0_2	[0.7-0.92]	R4_1
f2	f4_2_2	[0.9308-0.9644]	R5_1
f3	f4_3_2	(0.9644-0.9896]	R6_1
f4	f4_4_2	(0.9896-1.2]	R7_1
f5	f4_5_2		
f6	f4_6_2		
f7	f4_7_2		
f8	f4_8_2		
f11	f4_11_2		
f12	f4_12_2		
f13	f4_13_2		
f14	f4_14_2		
	X-element		
3p-shell		5s-shell	
p2	p3_2_3	s0	s5_0_3
p6	p3_6_3	s2	s5_2_3
3d-shell		5p-shell	
d0	d3_0_3	p0	p5_0_3
d2	d3_2_3	p2	p5_2_3

Feature	Gradation	Feature	Gradation
d10	d3_10_3	p6	p5_6_3
4s-shell		5d-shell	
s0	s4_0_3	d0	d5_0_3
s2	s4_2_3	d2	d5_2_3
4p-shell		d10	d5_10_3
p0	p4_0_3	6s-shell	
p2	p4_2_3	s0	s6_0_3
p6	p4_6_3	s2	s6_2_3
4d-shell		Ionic	
d0	d4_0_3	radius, A	
d2	d4_2_3	[0.39-0.4029]	R1_3
d10	d4_10_3	[0.4287-0.4502]	R2_3
4f-shell		[0.64-0.6824]	R3_3
f0	f4_0_3	[0.8114-0.82]	R4_3
f14	f4_14_3		

2.2.2.2.2. FEATURE SET 2.2.2.2

The second feature set (feature set 2.2.2.2) includes the following information: the first three ionization potentials, the electronegativities by Pauling, the entropies of the individual substances at 298 K, the isobaric thermal capacities at 298 K, the temperatures and the heats of melting and boiling, Debye (characteristic) temperatures, the energies of the crystal lattice, the ionic radii by Bokii and Belov, the ratio of the atomic number to the average atomic mass for atoms of elements A, B and X. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.2.2.2.2.1 contains the gradations for Feature Set 2.2.2.2.

Table 2.2.2.2.2.1

Gradations for Feature Set 2.2.2.2

Feature	Gradation	Feature	Gradation
	A-element		
First ionization potential, eV		Boiling point, K	
		[630-1226.319]	Tb_1_1
[5.21166-5.337139]	I1_1_1	[1351.572-1414.198]	Tb_2_1
[5.588098-5.79723]	I1_2_1	[1633.388-1696.015]	Tb_3_1
[6.048188-6.82]	I1_3_1	[1727.328-1880]	Tb_4_1
[7.344-7.9024]	I1_4_1	[2018-2350]	Tb_5_1

Feature	Gradation	Feature	Gradation
[8.9939-9.352474]	I1_5_1	[2698.031-3680]	Tb_6_1
(9.352474-10.4376]	I1_6_1	Heat of melting, kJ/mol	
Second ionization potential, eV		[2.295-7.22178]	Hm_1_1
[10.004-10.25021]	I2_1_1	(7.22178-7.38495]	Hm_2_1
[10.90677-11.23505]	I2_2_1	[7.95-8.47275]	Hm_3_1
[11.72747-12.05575]	I2_3_1	(8.47275-8.69031]	Hm_4_1
[13.58-16.908]	I2_4_1	[12.05-31.81968]	Hm_5_1
[17.084-18.12893]	I2_5_1	Heat of boiling, kJ/mol	
(18.12893-20.293]	I2_6_1	[59.229-121.2908]	Hb_1_1
Third ionization potential, eV		[137.2369-147.2032]	Hb_2_1
[27.49-39.343]	I3_1_1	(147.2032-157.737]	Hb_3_1
(39.343-41.705]	I3_2_1	[161.156-226.773]	Hb_4_1
(41.705-45.248]	I3_3_1	[296.102-444.759]	Hb_5_1
[47.61-53.515]	I3_4_1	Energy of the crystal lattice, -6 E*10 J/kg*mol	
[77.135-83.04]	I3_5_1		
[151.538-153.9]	I3_6_1		
Electronegativity		[116-137.203]	E_1_1
[0.9-0.921]	X_1_1	[144.807-154.312]	E_2_1
[0.991-1.019]	X_2_1	[161.916-169.52]	E_3_1
[1.187-1.215]	X_3_1	[173.322-180.926]	E_4_1
[1.481-1.516]	X_4_1	[188.53-200]	E_5_1
[1.586-1.9]	X_5_1	[286-503]	E_6_1
Entropies of individual substances at 298 K kJ/kg*mol*K		Debye temperature, K	
		[75-126.95]	Td_1_1
[9.498-11.08707]	S_1_1	(126.95-158.9]	Td_2_1
[23.64-33.86374]	S_2_1	[190-244.1]	Td_3_1
[40.22002-44.141]	S_3_1	[286.7-343]	Td_4_1
[51.75-79.898]	S_4_1	[370-585]	Td_5_1
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		[1138.7-1160]	Td_6_1
		Ratio of the atomic number to the average atomic mass	
[16.443-16.79196]	Cp_1_1		
[23.346-25.167]	Cp_2_1		
(25.167-25.7486]	Cp_3_1	[0.39-0.4127]	NM_1_1
(25.7486-26.276]	Cp_4_1	[0.42-0.4325]	NM_2_1
[26.443-27.02812]	Cp_5_1	[0.4379-0.4424]	NM_3_1
[27.72604-29.288]	Cp_6_1	[0.45-0.47]	NM_4_1
Melting point, K		[0.48-0.4919]	NM_5_1
[234.29-718.719]	Tm_1_1	[0.4973-0.5]	NM_6_1

Feature	Gradation	Feature	Gradation
[909.525-944.217]	Tm_2_1	Ionic radius, A	
[978.909-1022.274]	Tm_3_1	[0.34-0.3712]	Rb_1_1
(1022.274-1065.639]	Tm_4_1	[0.65-0.78]	Rb_2_1
[1100.331-1357]	Tm_5_1	[0.8-0.91]	Rb_3_1
[1533.981-2190]	Tm_6_1	[0.99-1.068]	Rb_4_1
		[1.12-1.26]	Rb_5_1
		[1.3488-1.44]	Rb_6_1
	B-element		
First ionization potential, eV		Boiling point, K	
[5.2-5.454721]	I1_1_2	[885-1825]	Tb_1_2
(5.454721-5.627047]	I1_2_2	[1903.31-2046.53]	Tb_2_2
(5.627047-5.741931]	I1_3_2	[2297-2547.8]	Tb_3_2
[5.7864-5.971699]	I1_4_2	(2547.8-2786.5]	Tb_4_2
(5.971699-6.00042]	I1_5_2	(2786.5-2858.11]	Tb_5_2
(6.00042-6.144025]	I1_6_2	(2858.11-2953.59]	Tb_6_2
(6.144025-6.172746]	I1_7_2	[3049.07-3216.16]	Tb_7_2
(6.172746-6.201467]	I1_8_2	(3216.16-3287.77]	Tb_8_2
(6.201467-6.266]	I1_9_2	(3287.77-3508]	Tb_9_2
[6.4-6.82]	I1_10_2	[3598.08-3743]	Tb_10_2
[7.2853-7.982169]	I1_11_2	[3932.26-4500]	Tb_11_2
[8.211937-9.789]	I1_12_2	Heat of melting, kJ/mol	
Second ionization potential, eV		[2.8-5.999477]	Hm_1_2
		[9.006855-9.963747]	Hm_2_2
[10.6-11.1822]	I2_1_2	(9.963747-10.37384]	Hm_3_2
(11.1822-12.0555]	I2_2_2	(10.37384-10.64724]	Hm_4_2
(12.0555-12.20105]	I2_3_2	(10.64724-10.78394]	Hm_5_2
(12.20105-12.8]	I2_4_2	(10.78394-11.05734]	Hm_6_2
[13.511-14.66]	I2_5_2	(11.05734-11.19404]	Hm_7_2
[15.64-17.084]	I2_6_2	(11.19404-12.5604]	Hm_8_2
[18.08-19.18745]	I2_7_2	[13.51792-14.6538]	Hm_9_2
[20.35185-20.93405]	I2_8_2	[15.062-15.8418]	Hm_10_2
[24.71835-25.155]	I2_9_2	[16.1152-16.662]	Hm_11_2
Third ionization potential, eV		[16.9354-17.48219]	Hm_12_2
		[18.02899-18.71248]	Hm_13_2
[18.3-19.74253]	I3_1_2	[18.98588-52]	Hm_14_2
[20-20.86759]	I3_2_2	Heat of boiling, kJ/mol	
(20.86759-21.43012]	I3_3_2		
(21.43012-21.80514]	I3_4_2	[31.798-191.6268]	Hb_1_2
(21.80514-21.99265]	I3_5_2	[205.4295-215.7815]	Hb_2_2
(21.99265-22.55518]	I3_6_2	(215.7815-227.61]	Hb_3_2
(22.55518-24.24277]	I3_7_2	[230-250.2883]	Hb_4_2

Feature	Gradation	Feature	Gradation
[24.61779-25.56]	I3_8_2	(250.2883-264.091]	Hb_5_2
[27.49-29.85]	I3_9_2	[284.7951-295.1472]	Hb_6_2
[30.4306-33.67]	I3_10_2	(295.1472-319.3019]	Hb_7_2
[37.55598-37.931]	I3_11_2	(319.3019-329.654]	Hb_8_2
Electronegativity		[338.293-364.1607]	Hb_9_2
[1.1-1.127]	X_1_2	[371.0621-385.186]	Hb_10_2
[1.181-1.3]	X_2_2	[410.45-468.922]	Hb_11_2
[1.478-1.523]	X_3_2	[490.693-512.54]	Hb_12_2
[1.577-1.622]	X_4_2	Energy of the	
[1.7-1.82]	X_5_2	crystal lattice,	
[1.9-2.2]	X_6_2	-6	
Entropies of		E*10 J/kg*mol	
individual		[182.8-286]	E_1_2
substances at 298 K		[312.419-337.5]	E_2_2
kJ/kg*mol*K		[356.1-368.327]	E_3_2
[5.853-7.921954]	S_1_2	(368.327-372.986]	E_4_2
[23.64-27.92184]	S_2_2	[390-407.152]	E_5_2
(27.92184-32.008]	S_3_2	(407.152-411.811]	E_6_2
[35.606-43.09417]	S_4_2	[427.341-578.5]	E_7_2
[44.47347-47.92173]	S_5_2	Debye	
(47.92173-51.91632]	S_6_2	temperature, K	
[53.42357-58.95615]	S_7_2	[89-127.75]	Td_1_2
[61.71475-64.47336]	S_8_2	(127.75-139]	Td_2_2
(64.47336-67.92162]	S_9_2	(139-161.5]	Td_3_2
(67.92162-72.74917]	S_10_2	(161.5-195.25]	Td_4_2
(72.74917-74.12847]	S_11_2	(195.25-251.5]	Td_5_2
(74.12847-74.81812]	S_12_2	[291-364]	Td_6_2
Isobaric thermal		[380-442.75]	Td_7_2
capacity at 298 K,		(442.75-585]	Td_8_2
kJ/kg*mol*K		[1196.5-1219]	Td_9_2
[11.088-11.85063]	Cp_1_2	Ratio of the	
[20.786-24.81528]	Cp_2_2	atomic number	
(24.81528-25.83212]	Cp_3_2	to the average	
(25.83212-26.59475]	Cp_4_2	atomic mass	
(26.59475-26.84896]	Cp_5_2	[0.39-0.4024]	NM_1_2
(26.84896-27.10317]	Cp_6_2	[0.4088-0.412]	NM_2_2
(27.10317-27.35738]	Cp_7_2	[0.4184-0.4216]	NM_3_2
(27.35738-27.61158	Cp_8_2	[0.43-0.4416]	NM_4_2
(27.61158-28.12]	Cp_9_2	[0.45-0.4624]	NM_5_2
(28.12-31.2]	Cp_10_2	[0.4688-0.472]	NM_6_2
[36.00048-36.5089]	Cp_11_2	[0.4784-0.48]	NM_7_2
Melting point, K		Ionic radius, A	
[303-576]	Tm_1_2	[0.2-0.2252]	Rb_1_2

Feature	Gradation	Feature	Gradation
[882.13-981.98]	Tm_2_2	[0.5612-0.64]	Rb_2_2
[1061.86-1141.74]	Tm_3_2	[0.6536-0.7]	Rb_3_2
(1141.74-1341.44]	Tm_4_2	[0.75-0.92]	Rb_4_2
(1341.44-1406]	Tm_5_2	[0.9308-0.9644]	Rb_5_2
[1500-1621.02]	Tm_6_2	(0.9644-0.9896]	Rb_6_2
(1621.02-1760.81]	Tm_7_2	(0.9896-1.2]	Rb_7_2
(1760.81-1800.75]	Tm_8_2		
(1800.75-1860.66]	Tm_9_2		
[1900.6-1980.48]	Tm_10_2		
[2163-2300]	Tm_11_2		
	X-element		
First ionization potential, eV		Boiling point, K	
[6.634-6.679531]	I1_1_3	[2896-2955.82]	Tb_1_3
[6.770593-6.831301]	I1_2_3	[3075.46-3175.16]	Tb_2_3
[7.316965-7.377673]	I1_3_3	[3494.2-3600]	Tb_3_3
[7.863337-7.939222]	I1_4_3	[4570.96-4650.72]	Tb_4_3
[8.121346-10]	I1_5_3	[4850.12-4890]	Tb_5_3
Second ionization potential, eV		Heat of melting, kJ/mol	
[13.13-13.58]	I2_1_3	[4.64735-5.46252]	Hm_1_3
[14.5772-14.70584]	I2_2_3	[6.549413-7.90803]	Hm_2_3
[14.83448-14.99528]	I2_3_3	[13.88594-15.24456]	Hm_3_3
[15.89576-16.0244]	I2_4_3	[20.13558-21.49419]	Hm_4_3
[16.28168-16.346]	I2_5_3	[31.27623-31.81968]	Hm_5_3
Third ionization potential, eV		Heat of boiling, kJ/mol	
[23.1-23.544]	I3_1_3	[296.102-304.2896]	Hb_1_3
[27.49-30.759]	I3_2_3	[375.2494-410.45]	Hb_2_3
[33.201-33.756]	I3_3_3	[552.6487-569.024]	Hb_3_3
[33.978-34.2]	I3_4_3	Energy of the crystal lattice, -6 E*10 J/kg*mol	
Electronegativity			
[1.3-1.321]	X_1_3	[302-310.46]	E_1_3
[1.391-1.5]	X_2_3	[321.74-335.84]	E_2_3
[1.783-1.818]	X_3_3	[364.04-378.14]	E_3_3
[1.986-2]	X_4_3	[470-584]	E_4_3
Entropies of individual substances at 298 K kJ/kg*mol*K		Debye temperature, K	
		[190-204.4]	Td_1_3
[18.828-19.58739]	S_1_3	[252.4-271.6]	Td_2_3
[30.627-31.73763]	S_2_3	[300.4-319.6]	Td_3_3

Feature	Gradation	Feature	Gradation
[38.31901-39.58466]	S_3_3	[358-470]	Td_4_3
[43.12848-43.88787]	S_4_3	[660.4-670]	Td_5_3
(43.88787-44.141]	S_5_3	Ratio of the atomic number to the average atomic mass	
Isobaric thermal capacity at 298 K, kJ/kg*mol*K			
[20.041-20.21296]	Cp_1_3	[0.4-0.403]	NM_1_3
[23.30824-23.53752]	Cp_2_3	[0.417-0.422]	NM_2_3
[25.104-25.4864]	Cp_3_3	[0.438-0.46]	NM_3_3
[25.60104-25.773]	Cp_4_3	[0.498-0.5]	NM_4_3
Melting point, K		Ionic radius, A	
[505-564.85]	Tm_1_3	[0.39-0.4029]	Rb_1_3
[1163.35-1263.1]	Tm_2_3	[0.4287-0.46]	Rb_2_3
[1662.1-1741.9]	Tm_3_3	[0.64-0.6824]	Rb_3_3
[1941-2180.8]	Tm_4_3	[0.8114-0.82]	Rb_4_3
[2460.1-2500]	Tm_5_3		

2.1.2.2.3. FEATURE SET 2.2.2.3

The third set of properties of simple oxides (feature set 2.2.2.3) includes the following information of simple oxides AO, B_2O_3 and XO : melting and boiling points, standard enthalpy of formation, standard isobaric thermal capacities, standard entropies, standard Gibbs energy, effective ionic radii of correspoding cations by Bokii and Belov. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.2.2.2.3.1 contains the gradations for Feature Set 2.2.2.3.

Table 2.2.2.2.3.1

Gradations for Feature Set 2.2.2.3
(Properties of Simple Oxides)

Feature	Gradation	Feature	Gradation
	AO		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
[-2.769-103.2]	H_1_1	[6.11-7.5]	Cp_1_1
[123-132.7534]	H_2_1	[8.46-9.22]	Cp_2_1
[139.5522-142.9516]	H_3_1	[9.5404-9.7452]	Cp_3_1
(142.9516-144.9912]	H_4_1	[9.95-10.1548]	Cp_4_1
(144.9912-147.0308]	H_5_1	[10.43-10.94]	Cp_5_1
[149.7504-151.79]	H_6_1	[11.0764-13.2]	Cp_6_1
Standard Gibbs energy for simple oxides, kcal/mol		Melting point of simple oxides, K	
		[780-2272.75]	Tm_1_1
		(2272.75-2314]	Tm_2_1
		[2809-2842]	Tm_3_1
[-3.463-96.229]	G_1_1	(2842-2875]	Tm_4_1
[116.738-125.9836]	G_2_1	[2908-2941]	Tm_5_1
[132.743-135.4468]	G_3_1	[3056.5-3073]	Tm_6_1
(135.4468-137.4746]	G_4_1	Boiling point of simple oxides, K	
(137.4746-140.1783]	G_5_1		
[142.8821-144.234]	G_6_1	[1746-3157.8]	Tb_1_1
Standard entropy for corresponding simple oxides, cal/mol*K		[3853.8-3900.2]	Tb_2_1
		[4248.2-4283]	Tb_3_1
		Ionic radii, A	
[3.29-3.7073]	So_1_1	[0.34-0.3712]	Rb_1_1
[6.2111-9.3]	So_2_1	[0.65-0.7664]	Rb_2_1
[10.1059-10.8014]	So_3_1	[0.78-0.91]	Rb_3_1
[12.06-14.7]	So_4_1	[0.97-1.068]	Rb_4_1
[16.42-20]	So_5_1	[1.12-1.26]	Rb_5_1
		[1.3488-1.44]	Rb_6_1
	B_2O_3		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
[85-228.9]	H_1_2	[7.83-16.8]	Cp_1_2
		[18-23.4]	Cp_2_2

Feature	Gradation	Feature	Gradation
[255.916-266.284]	H_2_2	(23.4-25.2]	Cp_3_2
[272.6-310.348]	H_3_2	(25.2-25.8]	Cp_4_2
[362.7-406.252]	H_4_2	(25.8-27]	Cp_5_2
[420-432.172]	H_5_2	(27-28.8]	Cp_6_2
(432.172-442.54]	H_6_2	[73.2-75]	Cp_7_2
(442.54-452.908]	H_7_2	Melting point of simple oxides, K	
(452.908-455.5]	H_8_2	[583-1107]	Tm_1_2
Standard Gibbs energy for simple oxides, kcal/mol		[1590.31-1670.99]	Tm_2_2
		[1953.37-2183]	Tm_3_2
		[2240-2376.94]	Tm_4_2
[66.167-198.835]	G_1_2	[2457.62-2497.96]	Tm_5_2
[206-253.099]	G_2_2	(2497.96-2578.64]	Tm_6_2
[272.33-291.9897]	G_3_2	(2578.64-2618.98]	Tm_7_2
[342.029-384.0256]	G_4_2	(2618.98-2679.49]	Tm_8_2
[404.478-409.5911]	G_5_2	(2679.49-2719.83]	Tm_9_2
(409.5911-419.8173]	G_6_2	(2719.83-2740]	Tm_10_2
(419.8173-430.0435]	G_7_2	Boiling point of simple oxides, K	
(430.0435-442.1]	G_8_2	[730.2-2462.28]	Tb_1_2
Standard entropy for corresponding simple oxides, cal/mol*K		[2941-3049.8]	Tb_2_2
		[4442.44-4529.48]	Tb_3_2
		(4529.48-4573]	Tb_4_2
[12.7-13.453]	So_1_2	Ionic radii, A	
[18.48-20.983]	So_2_2	[0.2-0.2252]	Rb_1_2
[22.991-25.8]	So_3_2	[0.5612-0.64]	Rb_2_2
[26.4-29.015]	So_4_2	[0.6536-0.7]	Rb_3_2
[30.019-31.023]	So_5_2	[0.75-0.92]	Rb_4_2
[31.525-32.529]	So_6_2	[0.9308-0.9644]	Rb_5_2
[33.533-34.788]	So_7_2	(0.9644-0.9896]	Rb_6_2
(34.788-35.541]	So_8_2	(0.9896-1.2]	Rb_7_2
[36.043-37.047]	So_9_2		
(37.047-58.81]	So_10_2		
	XO_2		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
		[10.62-10.7334]	Cp_1_3
[138.66-142.5132]	H_1_3	[11.943-12.0942]	Cp_2_3
[214.4396-225.59]	H_2_3	[12.5478-12.699]	Cp_3_3

Feature	Gradation	Feature	Gradation
[259.3936-267.1] Standard Gibbs energy for simple oxides, kcal/mol	H_3_3	[13.15-13.5306]	Cp_4_3
		[14.2866-14.4] Melting point of simple oxides, K	Cp_5_3
		[1389-1439.82]	Tm_1_3
[124.253-128.1338]	G_1_3	[1846.38-1931.08]	Tm_2_3
[203.1626-212.383]	G_2_3	[2143-2320.7]	Tm_3_3
[247.145-253.613]	G_3_3	[2930.54-3015.24]	Tm_4_3
Standard entropy for corresponding simple oxides, cal/mol*K		[3049.12-3083] Boiling point of simple oxides, K	Tm_5_3
		[2603-2608.1]	Tb_1_3
[9.49-9.6307]	So_1_3	[2767.9-2773]	Tb_2_3
[9.9121-10.0997]	So_2_3	Ionic radii, A	
[11.9757-12.1633]	So_3_3	[0.39-0.4029]	Rb_1_3
[12.4447-12.6323]	So_4_3	[0.4287-0.4502]	Rb_2_3
[14.0393-14.18]	So_5_3	[0.64-0.6824]	Rb_3_3
		[0.8114-0.82]	Rb_4_3

2.2.2.3. COMPUTER LEARNING AND PREDICTION OF CRYSTAL STRUCTURE

The computer learning is carried out for three learning sets in which the compounds from Table 2.2.2.1.1 were described in terms of the sets of the component properties 2.2.2.1, 2.2.2.2 and 2.2.2.3. The system of concept formation CONFOR [18-20] was used for computer learning and prediction.

The tables of predictions of the crystal structure type for the compounds of composition $A_2^{II}X_2^{IV}B^{III}O_7$ (Tables 2.2.2.3.1-2.2.2.3.3) result from the comparison of the results of prediction with use of the descriptions in terms of the Features Sets 2.2.2.1, 2.2.2.2 and 2.2.2.3. The melilites with X = Sn^{4+}, Zr^{4+} and Hf^{4+} do not be predicted. The following designations are used:

M - melilite;
- - the crystal structure differing from those listed above;
* - the compound of composition A_2XBO_7 does not form.

The physical-chemical systems, which were investigated experimentally, were marked by round brackets. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. The designation "?" corresponds to the indeterminate result of predicting. According to our results the new melilites of the composition $A_2XB_2O_7$ (X = Sn, Zr, or Hf) do not form at normal pressure and room temperature. The number of predicted melilites among silicates, germanates and titanates is a great one (see Tables 2.2.2.3.1-2.2.2.3.3). These compounds hold the promise for searching for new EO materials.

Table 2.2.2.3.1

Table of Predictions of Crystal Structure Type

for Compounds of Composition $A_2^{II}Si_2^{IV}B_2^{III}O_7$

A / B	Be	Mg	Ca	Zn	Sr	Cd	Ba	Hg	Pb	Ra
Al	?	?	(M)	?	(M)	?		M	M	M
Sc	?	M	M	M	M	M		M	M	M
Ti	M	M	M	M	M	M		M	M	M
V	M	M	M	M	M	M		M	M	M
Cr	M	M	M	M	M	M		M	M	M
Mn	M	M	M	M	M	M		M	M	M
Fe	M	M	M	M	M	M		M	M	M
Co	M	M	M	M	M	M	*	M	M	M
Ga	M	M	(M)	M	M	M	(*)	M	M	M
As	M	M	M	M	M	M		M	M	M
Y	(M)	M	M	M	M	M		M	M	M
Rh	M	M	M	M	M	M		M	M	M
In	?	M	M	M	M	M		M	M	M
Sb	M	M	M	M	M	M		M	M	M
La	?	?	?	?	?	?	?	-	-	-
Ce	?	?	?	?	?	?	*	-	-	-
Pr	?	?	?	?	?	?	?	-	-	-
Nd	(M)	?	?	?	?	?	?	-	-	-

A / B	Be	Mg	Ca	Zn	Sr	Cd	Ba	Hg	Pb	Ra
Pm	M	M	M	M	M	M		M	M	M
Sm	(M)	M	M	M	M	M		M	M	M
Eu	(M)	M	M	M	M	M		M	M	M
Gd	(M)	M	M	M	M	M		M	M	M
Tb	(M)	M	M	M	M	M		M	M	M
Dy	(M)	M	M	M	M	M		M	M	M
Ho	(M)	M	M	M	M	M		M	M	M
Er	(M)	M	M	M	M	M		M	M	M
Tm	(M)	M	M	M	M	M		M	M	M
Yb	(M)	M	M	M	M	M		M	M	M
Lu	(M)	M	M	M	M	M		M	M	M
Ac	-	-	-	-	-	-		-	-	-
Pa	-	-	-	-	-	-		-	-	-
U	-	-	-	-	-	-		-	-	-

Table 2.2.2.3.2

Table of Predictions of Crystal Structure Type

for Compounds of Composition $A_2^{II}Ge_2^{IV}B_2^{III}O_7$

A / B	Be	Mg	Ca	Zn	Sr	Cd	Ba	Hg	Pb	Ra
Al	?	?	(M)	?	(M)	?	(*)	M	M	M
Sc	?	M	M	M	M	M		M	M	M
Ti	M	M	M	M	M	M		M	M	M
V	M	M	M	M	M	M		M	M	M
Cr	M	M	M	M	M	M		M	M	M
Mn	M	M	M	M	M	M		M	M	M
Fe	M	M	*	M	(M)	M	(M)	M	M	M
Co	M	M	M	M	M	M	*	M	M	M
Ga	M	M	(M)	M	(M)	M	(M)	M	M	M
As	M	M	M	M	M	M		M	M	M
Y	(M)	M	M	M	M	M		M	M	M
Rh	M	M	M	M	M	M		M	M	M
In	?	M	M	M	M	M		M	M	M
Sb	M	M	M	M	M	M		M	M	M
La	(M)	?	?	?	(M)	?	?	-	-	-
Ce	M	?	?	?	?	?	?	-	-	-
Pr	(M)	?	?	?	?	?	?	-	-	-
Nd	(M)	?	?	?	?	?	?	-	-	-

A / B	Be	Mg	Ca	Zn	Sr	Cd	Ba	Hg	Pb	Ra
Pm	M	M	M	M	M	M		M	M	M
Sm	(M)	M	M	M	M	M		M	M	M
Eu	(M)	M	M	M	M	M		M	M	M
Gd	(M)	M	M	M	M	M		M	M	M
Tb	(M)	M	M	M	M	M		M	M	M
Dy	(M)	M	M	M	M	M		M	M	M
Ho	(M)	M	M	M	M	M		M	M	M
Er	(M)	M	M	M	M	M		M	M	M
Tm	(M)	M	M	M	M	M		M	M	M
Yb	(M)	M	M	M	M	M		M	M	M
Lu	(M)	M	M	M	M	M		M	M	M
Tl							-			
Bi							-			
Ac	-	-	-	-	-	-	-	-	-	-
Th							-			
Pa	-	-	-	-	-	-	-	-	-	-
U	-	-	-	-	-	-	-	-	-	-
Np							-			
Pu							-			
Am							-			

Table 2.2.2.3.3

Table of Predictions of Crystal Structure Type

for Compounds of Composition $A_2^{II}Ti_2^{IV}B_2^{III}O_7$

A / C	Be	Mg	Ca	Zn	Sr	Cd	Ba	Hg	Pb	Ra
Al	?	?	M	?	M	?	*	?	?	?
Sc	?	M	M	?	M	M	*	?	?	?
Ti	M	M	M	?	M	M	*	?	?	?
V	M	M	M	?	M	M	*	?	?	?
Cr	M	M	M	?	M	M	*	?	?	?
Mn	M	M	M	?	M	M	*	?	?	?
Fe	M	M	M	?	M	M	*	?	?	?
Co	M	M	M	?	M	M	*	?	?	?
Ga	M	M	M	?	M	M	*	?	?	?
As	M	M	M	?	M	M	*	?	?	?
Y	M	M	M	?	M	M	*	?	?	?
Rh	M	M	M	?	M	M	*	?	?	?
In	?	M	M	?	M	M	*	?	?	?
Sb	M	M	M	?	M	M	*	?	?	?
La	?	-	-	-	-	-	-	-	-	-
Ce	?	-	-	-	-	-		-	-	-
Pr	?	-	-	-	-	-	-	-	-	-
Nd	?	-	-	-	-	-	-	-	-	-

AC	Be	Mg	Ca	Zn	Sr	Cd	Ba	Hg	Pb	Ra
Pm	M	M	M	?	M	M	*	?	?	?
Sm	M	M	M	?	M	M	*	?	?	?
Eu	M	M	M	?	M	M	*	?	?	?
Gd	M	M	M	?	M	M	*	?	?	?
Tb	M	M	M	?	M	M	*	?	?	?
Dy	M	M	M	?	M	M	*	?	?	?
Ho	M	M	M	?	M	M	*	?	?	?
Er	M	M	M	?	M	M	*	?	?	?
Tm	M	M	M	?	M	M	*	?	?	?
Yb	M	M	M	?	M	M	*	?	?	?
Lu	M	M	M	?	M	M	*	?	?	?
Tl	-	-	-	-	-	-		-	-	-
Bi	-	-	-	-	-	-		-	-	-
Ac	-	-	-	-	-	-		-	-	-
Th	-	-	-	-	-	-		-	-	-
Pa	-	-	-	-	-	-		-	-	-
U	-	-	-	-	-	-		-	-	-
Np	-	-	-	-	-	-		-	-	-
Pu	-	-	-	-	-	-		-	-	-
Am	-	-	-	-	-	-		-	-	-

2.3. PREDICTION OF NEW COMPOUNDS OF COMPOSITION $AD(BO_3)_3O_4$

In last years much attention has been concentrated on the search for compounds having polyfunctional properties: high EO, piezoelectric, nonlinear optical, and other important characteristics. The purposeful search for such crystals is carried out, in particular, among borates with skeleton structures. Compounds, $LnAl_3(BO_3)_4 : Nd^{3+}$ (Ln = Y or Gd), with hantite structure (space group R32, Z=3) attract the attention of experts on the laser materials already for a long time. These compounds have unique properties among laser crystals. For example, the quantum luminescence efficiency in self-activated crystals with neodymium concentration $5.4*10^{21}$ cm^{-3} is equal to not less 0.1 and the average attenuation factor of luminescence remains on the level of tens microseconds. Moreover crystals of these hantites are electrical and optical nonlinear that provides the operation of self-doubling of laser generation frequency [2,24,27-29].

The physical and chemical properties of borates with hantite structure are closely related with their crystal structure. For example, weak concentration quenching in $NdAl_3(BO_3)_4$ is determined by the record large distance (5.92 A) between the most nearest ions Nd^{3+} [28,29]. It is possible to recognize the layers of two kinds: L_{2n} and L_{2n+1} in the hantite structure. The layers of first kind, L_{2n}, are formed by pairs of D-octahedra connected by edges and incorporated to layer by B-triangles. The formula of layer is $[D_2B_2O_{10}]$ and its symmetry is higher than symmetry of each structure and can be described by group of symmetry C2/m. The layers of second kind, L_{2n+1}, are formed by A-trigonal prisms and D-octahedra connected by vertices to pillars located along axis "a"; the pillars are also connected by B-triangles. The formula of layer is $[ADB_2O_{10}]$, and its symmetry is C2. If two layers join in structure, 16 atoms of oxygen collectivize and the result is the compound with formula $AD_3B_4O_{12}$. In case of hantite the subsequent odd layers L_{2n+1} are formed from initial layer by symmet-

rical duplication of even layers L_{2n} by axes 2 [24].

Such outline of formation of borates polytypes causes that there are some high-temperature crystal modifications for compounds, for example, with composition $LnAl_3(BO_3)_4$ [24,29]. Thus the higher is crystallizing temperature, the more complicated are the polytypes. The strict ordered polytypes form at low-speed cooling and the disordered structure arises at large speed cooling on background of ordered hantite structure that results in the loss of nonlinear optical and laser properties.

Authors of papers [24,29] mentioned the importance of account of size factors for prediction of possibility of hantite structure formation for complicated borates and its stability at various conditions of crystallization. However the limits of existence of hantite structure did not be found.

2.3.1. DATA FOR COMPUTER LEARNING

The data for computer learning was extracted from our the cardfile on quaternary inorganic compound properties. On the base of analysis of these data it may be concluded that only compounds $AD_3(BO_3)_4$ with boron can crystallize in hantite structure (exception - hantite with composition $CaMg_3(CO_3)_4$). Therefore this structure at room state and normal pressure was predicted only for complicated borates. The table 2.3.1.1 contains a learning set.

Table 2.3.1.1

Learning Set for Prediction of the Crystal Structure Type of Compounds with Composition $AD_3(BO_3)_4$

Composition	Crystal type	Space group
YAl3B4O12	hantite	
PrAl3B4O12	hantite	
NdAl3B4O12	hantite	
SmAl3B4O12	hantite	
EuAl3B4O12	hantite	
GdAl3B4O12	hantite	
TbAl3B4O12	hantite	
DyAl3B4O12	hantite	

Composition	Crystal type	Space group
HoAl3B4O12	hantite	
ErAl3B4O12	hantite	
TmAl3B4O12	hantite	
YbAl3B4O12	hantite	
LuAl3B4O12	hantite	
CeSc3B4O12	hantite	
PrSc3B4O12	hantite	
NdSc3B4O12	hantite	
SmSc3B4O12	hantite	
EuSc3B4O12	hantite	
YCr3B4O12	hantite	
NdCr3B4O12	hantite	
SmCr3B4O12	hantite	
GdCr3B4O12	hantite	
YFe3B4O12,	hantite	
LaFe3B4O12	hantite	
CeFe3B4O12	hantite	
PrFe3B4O12	hantite	
NdFe3B4O12	hantite	
SmFe3B4O12	hantite	
EuFe3B4O12	hantite	
GdFe3B4O12	hantite	
TbFe3B4O12	hantite	
DyFe3B4O12	hantite	
HoFe3B4O12	hantite	
YGa3B4O12	hantite	
NdGa3B4O12	hantite	
SmGa3B4O12	hantite	
EuGa3B4O12	hantite	
GdGa3B4O12	hantite	
TbGa3B4O12	hantite	
DyGa3B4O12	hantite	
ScSc3B4O12	calcite	
TiTi3B4O12	calcite	
VV3B4O12	calcite	
CrCr3B4O12	calcite	
FeFe3B4O12	calcite	
GaGa3B4O12	calcite	
YY3B4O12	calcite	
RhRh3B4O12	calcite	
InIn3B4O12	calcite	
LuLu3B4O12	calcite	
TlTl3B4O12	calcite	

Composition	Crystal type	Space group
LaLa3B4O12	aragonite	
CeCe3B4O12	aragonite	
PrPr3B4O12	aragonite	
NdNd3B4O12	aragonite	
PmPm3B4O12	aragonite	
AmAm3B4O12	aragonite	
SmSm3B4O12	vaterite	
EuEu3B4O12	vaterite	
GdGd3B4O12	vaterite	
TbTb3B4O12	vaterite	
DyDy3B4O12	vaterite	
HoHo3B4O12	vaterite	
ErEr3B4O12	vaterite	
TmTm3B4O12	vaterite	
YbYb3B4O12	vaterite	
AlAl3B4O12		P6(3)/m, Z=12
LaSc3B4O12		C2/c
YBO3-LaBO3	without compound	
LaBO3-YBO3	without compound	
LaBO3-NdBO3	without compound	
NdBO3-LaBO3	without compound	
LaBO3-SmBO3	without compound	
SmBO3-LaBO3	without compound	
LaBO3-EuBO3	without compound	
EuBO3-LaBO3	without compound	
LaBO3-GdBO3	without compound	
GdBO3-LaBO3	without compound	
LaBO3-DyBO3	without compound	
DyBO3-LaBO3	without compound	
LaBO3-HoBO3	without compound	
HoBO3-LaBO3	without compound	
LaBO3-ErBO3	without compound	
ErBO3-LaBO3	without compound	
LaBO3-TmBO3	without compound	
TmBO3-LaBO3	without compound	
LaBO3-YbBO3	without compound	
YbBO3-LaBO3	without compound	
LaBO3-LuBO3	without compound	
LuBO3-LaBO3	without compound	
NdBO3-SmBO3	without compound	
SmBO3-NdBO3	without compound	

2.3.2. SELECTION OF FEATURES

On the basis of physical-chemical grounds two sets of chemical elements features and set of simlpe oxides feature were selected for the description of these systems.

2.3.2.1. FEATURE SET 2.3.1

The first feature set (feature set 2.3.1) includes information about the number of electrons in energy shells of isolated atoms and Shannon effective ionic radii of elements A (C.N.=6) or D (C.N.=6) in the compound of composition $AD(BO_3)_4$. The grouping of energy shell information corresponds to the number of electrons for each shell. The quasi-continuous properties - the ionic radii - were divided using the special program of discretization [18]. Table 2.3.2.1.1 contains the gradations for Feature Set 2.3.1.

Table 2.3.2.1.1

Gradations for Feature Set 2.3.1

Feature	Gradation	Feature	Gradation
	A-element		
3p-shell		5s-shell	
p1	p3_0_1	s0	s5_0_1
p6	p3_6_1	s1	s5_1_1
3d-shell		s2	s5_2_1
d0	d3_0_1	5p-shell	
d1	d3_1_1	p0	p5_0_1
d2	d3_2_1	p1	p5_1_1
d3	d3_3_1	p3	p5_3_1
d5	d3_5_1	p6	p5_6_1
d6	d3_6_1	5d-shell	
d7	d3_7_1	d0	d5_0_1
d8	d3_8_1	d1	d5_1_1
d10	d3_10_1	d7	d5_7_1
4s-shell		d10	d5_10_1
s0	s4_0_1	5f-shell	
s1	s4_1_1	f0	f5_0_1
s2	s4_2_1	f2	f5_2_1
4p-shell		f3	f5_3_1
p0	p4_0_1	f4	f5_4_1
p1	p4_1_1	f6	f5_6_1
p3	p4_3_1	f7	f5_7_1
p6	p4_6_1	f8	f5_8_1

Feature	Gradation	Feature	Gradation
4d-shell		f10	f5_10_1
d0	d4_0_1	6s-shell	
d1	d4_1_1	s0	s6_0_1
d8	d4_8_1	s2	s6_2_1
d10	d4_10_1	6p-shell	
4f-shell		p0	p6_0_1
f0	f4_0_1	p1	p6_1_1
f2	f4_2_1	p3	p6_3_1
f3	f4_3_1	p6	p6_6_1
f4	f4_4_1	6d-shell	
f5	f4_5_1	d0	d6_0_1
f6	f4_6_1	d1	d6_1_1
f7	f4_7_1	7s-shell	
f8	f4_8_1	s0	s7_0_1
f10	f4_10_1	s2	s7_2_1
f11	f4_11_1	Ionic	
f12	f4_12_1	radius, A	
f13	f4_13_1	[0.27-0.54991]	Rs_1_1
f14	f4_14_1	[0.58-0.6841]	Rs_2_1
		[0.7338-0.76]	Rs_3_1
		[0.78847-0.81332]	Rs_4_1
		[0.85308-0.8829]	Rs_5_1
		(0.8829-0.88787]	Rs_6_1
		(0.88787-0.89781]	Rs_7_1
		(0.89781-0.9673899]	Rs_8_1
		(0.9673899-0.9822999]	Rs_9_1
		(0.9822999-1.00218]	Rs_10_1
		(1.00218-1.02206]	Rs_11_1
		(1.02206-1.12]	Rs_12_1
	D-element		
3p-shell		Ionic	
p1	p3_1_2	radius, A	
p6	p3_6_2	[0.27-0.54991]	Rs_1_1
3d-shell		[0.58-0.6344]	Rs_2_1
d0	d3_0_2	(0.6344-0.64434]	Rs_3_1
d1	d3_1_2	(0.64434-0.65925]	Rs_4_1
d2	d3_2_2	(0.65925-0.6841]	Rs_5_1
d3	d3_3_2	[0.7338-0.76	Rs_6_1
d5	d3_5_2	[0.78847-0.81332]	Rs_7_1
d6	d3_6_2	[0.85308-0.8829]	Rs_8_1
d7	d3_7_2	(0.8829-0.88787]	Rs_9_1
d8	d3_8_2	(0.88787-0.92266]	Rs_10_1

Feature	Gradation	Feature	Gradation
d10	d3_10_2	(0.92266-0.93757]	Rs_11_1
4s-shell		(0.93757-0.9673899]	Rs_12_1
s0	s4_0_2	(0.9673899-0.9822999]	Rs_13_1
s1	s4_1_2	(0.9822999-0.9872699]	Rs_14_1
s2	s4_2_2	(0.9872699-1.02206]	Rs_15_1
4p-shell		(1.02206-1.12]	Rs_16_1
p0	p4_0_2		
p1	p4_1_2		
p3	p4_3_2		
p6	p4_6_2		

2.3.2.2. FEATURE SET 2.3.2

The second feature set (feature set 2.3.2) includes the following information: the first three ionization potentials, the electronegativities by Pauling, the entropies of the individual substances at 298 K, the isobaric thermal capacities at 298 K, the temperatures and the heats of melting and boiling, Debye (characteristic) temperatures, the energies of the crystal lattice, the ionic radii by Shannon, the ratio of the atomic number to the average atomic mass for atoms of elements A, B and X. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.3.2.2.1 contains the gradations for Feature Set 2.3.2.

Table 2.3.2.2.1

Gradations for Feature Set 2.3.2

Feature	Gradation	Feature	Gradation
	A-element		
First ionization potential, eV		Boiling point, K	
		[885-1657.5]	Tb_1_1
[5.2-5.450764]	I1_1_1	(1657.5-1743.5]	Tb_2_1
(5.450764-5.525056]	I1_2_1	(1743.5-1825]	Tb_3_1
(5.525056-5.574584]	I1_3_1	[1894-1980]	Tb_4_1
(5.574584-5.624112]	I1_4_1	(1980-2044.5]	Tb_5_1
(5.624112-5.723168]	I1_5_1	[2259.5-2350]	Tb_6_1
(5.723168-5.846988]	I1_6_1	[2431.5-2539]	Tb_7_1
(5.846988-5.970808]	I1_7_1	(2539-2646.5]	Tb_8_1
(5.970808-5.995572]	I1_8_1	(2646.5-2732.5]	Tb_9_1
(5.995572-6.144156]	I1_9_1	(2732.5-2754]	Tb_10_1
(6.144156-6.16892]	I1_10_1	(2754-2775.5]	Tb_11_1

Feature	Gradation	Feature	Gradation
(6.16892-6.193684]	I1_11_1	(2775.5-2840]	Tb_12_1
(6.193684-6.243212]	I1_12_1	(2840-2883]	Tb_13_1
(6.243212-6.317504]	I1_13_1	(2883-2947.5]	Tb_14_1
[6.515616-6.614672]	I1_14_1	(2947.5-3012]	Tb_15_1
[6.713728-6.887076]	I1_15_1	(3012-3119.5]	Tb_16_1
[7.2853-7.637]	I1_16_1	(3119.5-3205.5]	Tb_17_1
[7.828108-9.789]	I1_17_1	[3230-3442]	Tb_18_1
Second ionization		(3442-3528]	Tb_19_1
potential, eV		[3571-3635.5]	Tb_20_1
[10.6-10.7983]	I2_1_1	(3635.5-3678.5]	Tb_21_1
(10.7983-10.89745]	I2_2_1	(3678.5-3721.5]	Tb_22_1
(10.89745-11.09575]	I2_3_1	(3721.5-4650]	Tb_23_1
(11.09575-11.1949]	I2_4_1	Heat of melting,	
(11.1949-11.7898]	I2_5_1	kJ/mol	
(11.7898-12.08725]	I2_6_1	[2.8-4.84384]	Hm_1_1
(12.08725-12.48385]	I2_7_1	[5.2388-6.02872]	Hm_2_1
[12.68215-13.07875]	I2_8_1	[8.79344-10.57076]	Hm_3_1
[13.47535-13.87195]	I2_9_1	(10.57076-10.76824]	Hm_4_1
(13.87195-14.1694]	I2_10_1	(10.76824-11.1632]	Hm_5_1
[14.3677-14.86345]	I2_11_1	(11.1632-11.75564]	Hm_6_1
[15.64-16.7473]	I2_12_1	[12.05-13.138]	Hm_7_1
[17.08-18.3337]	I2_13_1	[13.53296-14.32288]	Hm_8_1
[18.532-18.82945]	I2_14_1	(14.32288-14.91532]	Hm_9_1
(18.82945-19.1269]	I2_15_1	(14.91532-15.31028]	Hm_10_1
[20.3167-25.155]	I2_16_1	(15.31028-15.90272]	Hm_11_1
Third ionization		(15.90272-16.29768]	Hm_12_1
potential, eV		(16.29768-17.68004]	Hm_13_1
[19.18-19.5376]	I3_1_1	[18.075-19.65484]	Hm_14_1
[20.0144-20.4912]	I3_2_1	[20.085-22.0246]	Hm_15_1
(20.4912-20.8488]	I3_3_1	[22.41956-52]	Hm_16_1
(20.8488-21.2064]	I3_4_1	Heat of boiling,	
[21.4448-22.2792]	I3_5_1	kJ/mol	
(22.2792-22.6368]	I3_6_1	[31.798-174.0386]	Hb_1_1
(22.6368-22.756]	I3_7_1	(174.0386-180.6053]	Hb_2_1
(22.756-23.5904]	I3_8_1	(180.6053-190.4552]	Hb_3_1
(23.5904-23.948]	I3_9_1	[203.5885-223.2884]	Hb_4_1
[24.4248-24.7824]	I3_10_1	(223.2884-229.8551]	Hb_5_1
(24.7824-25.0208]	I3_11_1	(229.8551-239.705]	Hb_6_1
(25.0208-25.56]	I3_12_1	(239.705-249.555]	Hb_7_1
[27.2856-28.2392]	I3_13_1	(249.555-262.6883]	Hb_8_1
(28.2392-28.716]	I3_14_1	[288.9548-295.5215]	Hb_9_1
[28.9544-30.1464]	I3_15_1	(295.5215-328.3547]	Hb_10_1
[30.3848-37.931]	I3_16_1	[334.9213-354.6212]	Hb_11_1

Feature	Gradation	Feature	Gradation
Electronegativity		(354.6212-364.4712]	Hb_12_1
[1.1-1.133]	X_1_1	[369.866-385.186]	Hb_13_1
[1.177-1.232]	X_2_1	[403.871-417.0043]	Hb_14_1
[1.276-1.331]	X_3_1	(417.0043-426.8543]	Hb_15_1
[1.485-1.529]	X_4_1	[439.9875-460.548]	Hb_16_1
[1.573-1.628]	X_5_1	[485.954-612.538]	Hb_17_1
[1.672-1.727]	X_6_1	Energy of the	
[1.771-1.9]	X_7_1	crystal lattice,	
[2.178-2.2]	X_8_1	-6	
Entropies of		E*10 J/kg*mol	
individual		[182.8-208]	E_1_1
substances at 298 K		[234.241-254.4]	E_2_1
kJ/kg*mol*K		[269.854-286]	E_3_1
[5.853-25.17534]	S_1_1	[309.424-325.252]	E_4_1
[26.19891-28.24603]	S_2_1	[333.166-348.994]	E_5_1
(28.24603-28.75781]	S_3_1	(348.994-360.865]	E_6_1
(28.75781-32.85206]	S_4_1	(360.865-368.779]	E_7_1
[35.48-38.99343]	S_5_1	(368.779-380.65]	E_8_1
[40.017-42.5759]	S_6_1	(380.65-416.263]	E_9_1
[44.62303-47.18193]	S_7_1	[424.177-440.005]	E_10_1
[48.2055-51.91632]	S_8_1	[463.747-479.575]	E_11_1
[56.394-57.41756]	S_9_1	[495.403-524]	E_12_1
(57.41756-58.9529]	S_10_1	[566.629-641.5]	E_13_1
[62.02359-64.07072]	S_11_1	Debye	
(64.07072-65.60606]	S_12_1	temperature, K	
(65.60606-69.18853]	S_13_1	[89-93.96]	Td_1_1
(69.18853-70.72387]	S_14_1	(93.96-108.84]	Td_2_1
(70.72387-71.23565]	S_15_1	(108.84-118.76]	Td_3_1
(71.23565-71.74744]	S_16_1	(118.76-128.68]	Td_4_1
(71.74744-72.771]	S_17_1	(128.68-143.56]	Td_5_1
(72.771-74.81812]	S_18_1	(143.56-158.44]	Td_6_1
Isobaric thermal		(158.44-178.28]	Td_7_1
capacity at 298 K,		[200-232.84]	Td_8_1
kJ/kg*mol*K		[291-346.92]	Td_9_1
[11.088-23.74089]	Cp_1_1	[366.76-391.56]	Td_10_1
[24.00415-24.66229]	Cp_2_1	[411.4-426.28]	Td_11_1
(24.66229-25.05718]	Cp_3_1	(426.28-450]	Td_12_1
(25.05718-25.45206]	Cp_4_1	[461-490.76]	Td_13_1
[25.71532-25.97858]	Cp_5_1	[570.12-1219]	Td_14_1
(25.97858-26.76835]	Cp_6_1	Ratio of the	
(26.76835-27.82139]	Cp_7_1	atomic number	
(27.82139-28.08464]	Cp_8_1	to the average	
(28.08464-28.21627]	Cp_9_1	atomic mass	

Feature	Gradation	Feature	Gradation
(28.21627-31.2]	Cp_10_1	[0.39-0.3927]	NM_1_1
[36.24564-36.5089]	Cp_11_1	[0.3981-0.4026]	NM_2_1
Melting point, K		[0.408-0.4125]	NM_3_1
[303-360.99]	Tm_1_1	[0.4179-0.4224]	NM_4_1
[399.65-476.97]	Tm_2_1	[0.4278-0.4323]	NM_5_1
[544.5-631.61]	Tm_3_1	[0.4377-0.4422]	NM_6_1
[902.23-979.55]	Tm_4_1	[0.4476-0.4521]	NM_7_1
[1056.87-1095.53]	Tm_5_1	[0.4575-0.462]	NM_8_1
(1095.53-1153.52]	Tm_6_1	[0.4674-0.4719]	NM_9_1
(1153.52-1250.17]	Tm_7_1	[0.4773-0.48]	NM_10_1
(1250.17-1406]	Tm_8_1	Ionic radius, A	
[1500-1733.42]	Tm_9_1	[0.27-0.54991]	Rs_1_1
(1733.42-1772.08]	Tm_10_1	[0.58-0.6841]	Rs_2_1
(1772.08-1810.74]	Tm_11_1	[0.7338-0.76]	Rs_3_1
(1810.74-1868.73]	Tm_12_1	[0.78847-0.81332]	Rs_4_1
[1907.39-1984.71]	Tm_13_1	[0.85308-0.8829]	Rs_5_1
[2139.35-2720]	Tm_14_1	(0.8829-0.88787]	Rs_6_1
		(0.88787-0.89781]	Rs_7_1
		(0.89781-0.9673899]	Rs_8_1
		(0.9673899-0.9822999]	Rs_9_1
		(0.982299901.00218]	Rs_10_1
		(1.0021801.02206]	Rs_11_1
		(1.0220601.12]	Rs_12_1
	D-element		
First ionization potential, eV		Boiling point, K	
[5.2-5.450764]	I1_1_2	[885-1743.5]	Tb_1_2
(5.450764-5.500292]	I1_2_2	(1743.5-1825]	Tb_2_2
(5.500292-5.525056]	I1_3_2	[1894-2044.5]	Tb_3_2
(5.525056-5.574584]	I1_4_2	[2259.5-2350]	Tb_4_2
(5.574584-5.624112]	I1_5_2	[2431.5-2539]	Tb_5_2
(5.624112-5.723168]	I1_6_2	(2539-2732.5]	Tb_6_2
(5.723168-5.846988]	I1_7_2	(2732.5-2754]	Tb_7_2
(5.846988-5.92128]	I1_8_2	(2754-2775.5]	Tb_8_2
(5.92128-5.970808]	I1_9_2	(2775.5-2840]	Tb_9_2
(5.970808-6.020336]	I1_10_2	(2840-2883]	Tb_10_2
(6.020336-6.317504]	I1_11_2	(2883-3012]	Tb_11_2
[6.515616-6.614672]	I1_12_2	(3012-3119.5]	Tb_12_2
[6.713728-6.763256]	I1_13_2	(3119.5-3205.5]	Tb_13_2
(6.763256-6.812784]	I1_14_2	[3230-3442]	Tb_14_2
(6.812784-7.5763]	I1_15_2	(3442-3528]	Tb_15_2
[7.36-7.53094]	I1_16_2	[3571-3635.5]	Tb_16_2
		(3635.5-3678.5]	Tb_17_2

Feature	Gradation	Feature	Gradation
[7.6-9.789]	I1_17_2	(3678.5-3721.5]	Tb_18_2
Second ionization		(3721.5-5770]	Tb_19_2
potential, eV		Heat of melting,	
[10.6-10.69915]	I2_1_2	kJ/mol	
(10.69915-10.7983]	I2_2_2	[2.8-4.84384]	Hm_1_2
(10.7983-11.09575]	I2_3_2	[5.2388-6.02872]	Hm_2_2
(11.09575-11.1949]	I2_4_2	[8.79344-9.78084]	Hm_3_2
(11.1949-11.49235]	I2_5_2	(9.78084-10.37328]	Hm_4_2
(11.49235-11.69065]	I2_6_2	(10.37328-10.57076]	Hm_5_2
(11.69065-12.48385]	I2_7_2	(10.57076-10.76824]	Hm_6_2
[12.68215-13.07875]	I2_8_2	(10.76824-11.1632]	Hm_7_2
[13.47535-13.87195]	I2_9_2	(11.1632-11.75564]	Hm_8_2
(13.87195-14.1694]	I2_10_2	[12.04-13.138]	Hm_9_2
[14.31-14.86345]	I2_11_2	[13.53296-14.32288]	Hm_10_2
[15.63-16.76]	I2_12_2	(14.32288-14.91532]	Hm_11_2
[17.08-18.3337]	I2_13_2	(14.91532-15.31028]	Hm_12_2
[18.532-18.82945]	I2_14_2	(15.31028-15.90272]	Hm_13_2
(18.82945-19.43]	I2_15_2	(15.90272-16.29768]	Hm_14_2
[20.292-25.155]	I2_16_2	(16.29768-16.89012]	Hm_15_2
Third ionization		(16.89012-17.68004]	Hm_16_2
potential, eV		[18.075-20.085]	Hm_17_2
[19.18-19.5376]	I3_1_2	[20.44476-21.43216]	Hm_18_2
[20.0144-20.4912]	I3_2_2	(21.43216-22.0246]	Hm_19_2
(20.4912-21.2064]	I3_3_2	[22.41956-52]	Hm_20_2
[21.4448-21.8024]	I3_4_2	Heat of boiling,	
(21.8024-22.0408]	I3_5_2	kJ/mol	
(22.0408-22.2792]	I3_6_2	[31.798-174.0386]	Hb_1_2
(22.2792-22.6368]	I3_7_2	(174.0386-180.6053]	Hb_2_2
(22.6368-23.948]	I3_8_2	(180.6053-190.4552]	Hb_3_2
[24.4248-24.7824]	I3_9_2	[203.5885-223.2884]	Hb_4_2
(24.7824-25.56]	I3_10_2	(223.2884-229.8551]	Hb_5_2
[27.2-28.2392]	I3_11_2	(229.8551-239.705]	Hb_6_2
(28.2392-28.716]	I3_12_2	(239.705-249.555]	Hb_7_2
[28.9544-30.1464]	I3_13_2	(249.555-262.6883]	Hb_8_2
[30.3848-37.931]	I3_14_2	[288.9548-295.5215]	Hb_9_2
Electronegativity		(295.5215-298.8048]	Hb_10_2
[1.1-1.133]	X_1_2	(298.8048-308.6548]	Hb_11_2
[1.177-1.232]	X_2_2	(308.6548-318.5047]	Hb_12_2
[1.276-1.331]	X_3_2	(318.5047-330.954]	Hb_13_2
[1.485-1.529]	X_4_2	[334.9213-354.6212]	Hb_14_2
[1.573-1.628]	X_5_2	(354.6212-364.4712]	Hb_15_2
[1.672-1.727]	X_6_2	[369-385.186]	Hb_16_2
[1.771-1.9]	X_7_2	[403.871-417.0043]	Hb_17_2

Feature	Gradation	Feature	Gradation
[2.178-2.4]	X_8_2	(417.0043-426.8543]	Hb_18_2
Entropies of		[439.9875-460.548]	Hb_19_2
individual		[485.954-744.752]	Hb_20_2
substances at 298 K		Energy of the	
kJ/kg*mol*K		crystal lattice,	
[5.853-25.17534]	S_1_2	-6	
[26.19891-28.75781]	S_2_2	E*10 J/kg*mol	
(28.75781-32.85206]	S_3_2	[25.2-208]	E_1_2
[33.1-38.99343]	S_4_2	[234.241-254.4]	E_2_2
[40.017-42.5759]	S_5_2	[269.854-290]	E_3_2
[44.62303-47.405]	S_6_2	[309.424-325.252]	E_4_2
[48.2055-51.91632]	S_7_2	[333.166-348.994]	E_5_2
[56.394-57.41756]	S_8_2	(348.994-360.865]	E_6_2
(57.41756-58.9529]	S_9_2	(360.865-380.65]	E_7_2
[62.02359-64.07072]	S_10_2	(380.65-416.263]	E_8_2
(64.07072-65.60606]	S_11_2	[424.177-440.005]	E_9_2
(65.60606-69.18853]	S_12_2	[463.747-479.575]	E_10_2
(69.18853-70.72387]	S_13_2	[495.403-524]	E_11_2
(70.72387-71.74744]	S_14_2	[566.629-775]	E_12_2
(71.74744-72.771]	S_15_2	Debye	
(72.771-74.81812]	S_16_2	temperature, K	
Isobaric thermal		[89-93.96]	Td_1_2
capacity at 298 K,		(93.96-108.84]	Td_2_2
kJ/kg*mol*K		(108.84-118.76]	Td_3_2
[11.088-23.74089]	Cp_1_2	(118.76-128.68]	Td_4_2
[24.00415-24.66229]	Cp_2_2	(128.68-148.52]	Td_5_2
(24.66229-24.92555]	Cp_3_2	(148.52-178.28]	Td_6_2
(24.92555-25.45206]	Cp_4_2	[200-250]	Td_7_2
[25.71532-25.97858]	Cp_5_2	[275-346.92]	Td_8_2
(25.97858-26.24184]	Cp_6_2	[366.76-391.56]	Td_9_2
(26.24184-26.76835]	Cp_7_2	[411.4-426.28]	Td_10_2
(26.76835-27.29487]	Cp_8_2	(426.28-450]	Td_11_2
(27.29487-27.4265]	Cp_9_2	[461-475.88]	Td_12_2
(27.4265-27.82139]	Cp_10_2	(475.88-490.76]	Td_13_2
(27.82139-28.08464]	Cp_11_2	[570.12-1219]	Td_14_2
(28.08464-31.2]	Cp_12_2	Ratio of the	
[36.24564-36.5089]	Cp_13_2	atomic number	
Melting point, K		to the average	
[303-360.99]	Tm_1_2	atomic mass	
[399.65-476.97]	Tm_2_2	[0.39-0.3927]	NM_1_2
[544.5-631.61]	Tm_3_2	[0.3981-0.4026]	NM_2_2
[902.23-979.55]	Tm_4_2	[0.408-0.4125]	NM_3_2
[1056.87-1095.53]	Tm_5_2	[0.4179-0.4224]	NM_4_2

Feature	Gradation	Feature	Gradation
(1095.53-1153.52]	Tm_6_2	[0.4278-0.4323]	NM_5_2
(1153.52-1250.17]	Tm_7_2	[0.4377-0.4422]	NM_6_2
(1250.17-1406]	Tm_8_2	[0.4476-0.4521]	NM_7_2
[1500-1617.44]	Tm_9_2	[0.4575-0.462]	NM_8_2
(1617.44-1675.43]	Tm_10_2	[0.4674-0.4719]	NM_9_2
(1675.43-1810.74]	Tm_11_2	[0.4773-0.48]	NM_10_2
(1810.74-1868.73]	Tm_12_2	Ionic radius, A	
[1907.39-1984.71]	Tm_13_2	[0.27-0.54991]	Rs_1_2
[2139.35-2178.01]	Tm_14_2	[0.58-0.6344]	Rs_2_2
(2178.01-3287]	Tm_15_2	(0.6344-0.64434]	Rs_3_2
		(0.64434-0.65925]	Rs_4_2
		(0.65925-0.69]	Rs_5_2
		[0.72-0.76]	Rs_6_2
		[0.78847-0.81332]	Rs_7_2
		[0.85-0.8829]	Rs_8_2
		(0.8829-0.88787]	Rs_9_2
		(0.88787-0.92266]	Rs_10_2
		(0.92266-0.93757]	Rs_11_2
		(0.93757-0.9673899]	Rs_12_2
		(0.9673899-0.9822999]	Rs_13_2
		(0.9822999-0.9872699]	Rs_14_2
		(0.9872699-1.02206]	Rs_15_2
		(1.02206-1.12]	Rs_16_2

2.3.2.3. FEATURE SET 2.3.3

The third set of properties of simple oxides (feature set 2.3.3) includes the following information of simple oxides A_2O_3 and D_2O_3: the melting and boiling points, standard enthalpy of formation, standard isobaric thermal capacities, standard entropies, standard Gibbs energy, effective ionic radii of correspoding cations by Shannon. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.3.2.3.1 contains the gradations for Feature Set 2.3.3.

Table 2.3.2.3.1

Gradations for Feature Set 2.3.3
(Properties of Simple Oxides)

Feature	Gradation	Feature	Gradation
	A O 2 3		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
[85-103.525]	H_1_1	[7.83-14.084]	Cp_1_1
[138.1-207.265]	H_2_1	[17.852-20.364]	Cp_2_1
[214.675-229.495]	H_3_1	(20.364-24.132]	Cp_3_1
[251.725-304.23]	H_4_1	(24.132-26.016]	Cp_4_1
[351.76-370.285]	H_5_1	(26.016-27.272]	Cp_5_1
[387-411.04]	H_6_1	(27.272-27.9]	Cp_6_1
(411.04-429.565]	H_7_1	(27.9-29.784]	Cp_7_1
(429.565-433.27]	H_8_1	[73.744-75]	Cp_8_1
(433.27-444.385]	H_9_1	Melting point of simple oxides, K	
(444.385-451.795]	H_10_1	[583-1155.99]	Tm_1_1
(451.795-455.5]	H_11_1	[1580.57-1662.22]	Tm_2_1
Standard Gibbs energy for simple oxides, kcal/mol		[1923.5-1988.82]	Tm_3_1
		(1988.82-2037.81]	Tm_4_1
		[2070.47-2282.76]	Tm_5_1
		(2282.76-2364.41]	Tm_6_1
[66.167-84.96365]	G_1_1	[2429.73-2478.72]	Tm_7_1
[118.867-186.4656]	G_2_1	(2478.72-2527.71]	Tm_8_1
[193.9842-205.2622]	G_3_1	(2527.71-2560.37]	Tm_9_1
(205.2622-216.5402]	G_4_1	(2560.37-2576.7]	Tm_10_1
[231.5775-285.325]	G_5_1	(2576.7-2593.03]	Tm_11_1
[333.0794-351.8761]	G_6_1	(2593.03-2658.35]	Tm_12_1
[366.9134-385.7101]	G_7_1	(2658.35-2674.68]	Tm_13_1
[400.7474-408.266]	G_8_1	(2674.68-2723.67]	Tm_14_1
(408.266-427.0627]	G_9_1	(2723.67-2740]	Tm_15_1
(427.0627-430.822]	G_10_1	Boiling point of simple oxides, K	
(430.822-438.3407]	G_11_1	[730.2-3047.19]	Tb_1_1
(438.3407-442.1]	G_12_1	[4431.43-4510.08]	Tb_2_1
Standard entropy for corresponding simple oxides, cal/mol*K		[4541.54-4573]	Tb_3_1
		Ionic radii, A	
[12.7-13.453]	So_1_1	[0.27-0.54991]	Rs_1_1
[17.971-20.983]	So_2_1	[0.58-0.6841]	Rs_2_1
		[0.7338-0.76]	Rs_3_1

Feature	Gradation	Feature	Gradation
[22.991-23.493]	So_3_1	[0.78847-0.81332]	Rs_4_1
(23.493-24.246]	So_4_1	[0.85308-0.8829]	Rs_5_1
[24.748-26.505]	So_5_1	(0.8829-0.88787]	Rs_6_1
[27.89-29.015]	So_6_1	(0.88787-0.89781]	Rs_7_1
[30.019-31.023]	So_7_1	(0.89781-0.9673899]	Rs_8_1
[31.525-32.529]	So_8_1	(0.9673899-0.9822999]	Rs_9_1
[33.533-35.29]	So_9_1	(0.9822999-1.00218]	Rs_10_1
(35.29-36.043]	So_10_1	(1.00218-1.02206]	Rs_11_1
(36.043-36.796]	So_11_1	(1.02206-1.12]	Rs_12_1
(36.796-37.047]	So_12_1		
(37.047-37.298]	So_13_1		
(37.298-37.549]	So_14_1		
(37.549-58.81]	So_15_1		
	D O 2 3		
Standard enthalpy of formation for corresponding simple oxides, kcal/mol		Standard isobaric thermal capacity for simple oxides, cal/mol*K	
		[7.83-14.084]	Cp_1_2
[85-138.1]	H_1_2	[17.852-22.876]	Cp_2_2
[157-207.265]	H_2_2	(22.876-24.132]	Cp_3_2
[214.675-229.495]	H_3_2	(24.132-26.016]	Cp_4_2
[251.725-281.365]	H_4_2	(26.016-27.272]	Cp_5_2
(281.365-304.23]	H_5_2	(27.272-27.9]	Cp_6_2
[351.76-370.285]	H_6_2	(27.9-29.784]	Cp_7_2
[387-411.04]	H_7_2	[73.744-75]	Cp_8_2
(411.04-429.565]	H_8_2	Melting point of simple oxides, K	
(429.565-433.27]	H_9_2		
(433.27-444.385]	H_10_2	[583-1155.99]	Tm_1_2
(444.385-451.795]	H_11_2	[1580.57-1662.22]	Tm_2_2
(451.795-455.5]	H_12_2	[1923.5-1988.82]	Tm_3_2
Standard Gibbs energy for simple oxides, kcal/mol		(1988.82-2037.81]	Tm_4_2
		[2070.47-2282.76]	Tm_5_2
		(2282.76-2364.41]	Tm_6_2
		[2429.73-2478.72]	Tm_7_2
[66.167-118.867]	G_1_2	(2478.72-2560.37]	Tm_8_2
[137.7-186.4656]	G_2_2	(2560.37-2576.7]	Tm_9_2
[193.9842-205.2622]	G_3_2	(2576.7-2593.03]	Tm_10_2
(205.2622-216.5402]	G_4_2	(2593.03-2609.36]	Tm_11_2
[231.5775-261.6522]	G_5_2	(2609.36-2674.68]	Tm_12_2
(261.6522-285.325]	G_6_2	(2674.68-2723.67]	Tm_13_2

Feature	Gradation	Feature	Gradation
[333.0794-351.8761]	G_7_2	(2723.67-2740]	Tm_14_2
[366.9134-385.7101]	G_8_2	Boiling point of	
[400.7474-412.0254]	G_9_2	simple oxides, K	
(412.0254-438.3407]	G_10_2	[730.2-3047.19]	Tb_1_2
(438.3407-442.1]	G_11_2	[4431.43-4510.08]	Tb_2_2
Standard entropy		[4541.54-4573]	Tb_3_2
for corresponding		Ionic radii, A	
simple oxides,		[0.27-0.54991]	Rs_1_2
cal/mol*K		[0.58-0.6344]	Rs_2_2
[12.7-13.453]	So_1_2	(0.6344-0.64434]	Rs_3_2
[17.971-18.724]	So_2_2	(0.64434-0.65925]	Rs_4_2
(18.724-20.983]	So_3_2	(0.65925-0.6841]	Rs_5_2
[22.991-23.493]	So_4_2	[0.7338-0.76]	Rs_6_2
(23.493-24.246]	So_5_2	[0.78847-0.81332]	Rs_7_2
[24.748-26.505]	So_6_2	[0.85308-0.8829]	Rs_8_2
[27.89-29.015]	So_7_2	(0.8829-0.88787]	Rs_9_2
[30.019-31.023]	So_8_2	(0.88787-0.92266]	Rs_10_2
[31.525-32.529]	So_9_2	(0.92266-0.93757]	Rs_11_2
[33.533-34.286]	So_10_2	(0.93757-0.9673899]	Rs_12_2
(34.286-34.788]	So_11_2	(0.9673899-0.9822999]	Rs_13_2
(34.788-35.29]	So_12_2	(0.9822999-0.9872699]	Rs_14_2
(35.29-36]	So_13_2	(0.9872699- 1.02206]	Rs_15_2
[36.043-36.796]	So_14_2	(1.02206-1.12]	Rs_16_2
(36.796-37.047]	So_15_2		
(37.047-37.298]	So_16_2		
(37.298-37.549]	So_17_2		
(37.549-58.81]	So_18_2		

2.3.3. COMPUTER LEARNING AND PREDICTION OF CRYSTAL STRUCTURE

The computer learning is carried out for three learning sets in which the compounds from Table 2.3.1.1 were described in terms of the sets of the component properties 2.3.1, 2.3.2 and 2.3.3. The system of concept formation CONFOR [18-20] was used for computer learning and prediction.

The table of predictions of the crystal structure type for the compounds of composition $AD(BO_4)_3$ (Table 2.3.3.1) results from the comparison of the results of prediction with use of the descriptions in terms of the Features Sets 2.3.1, 2.3.2 and 2.3.3. The following designations are used:

H - hantite;
C - calcite (space group R3(-)c, Z=3);
A - aragonite (space group Pbnm, Z=4);
- - the crystal structure differing from those listed above;
* - the compound of composition $AD(BO_3)_4$ does not form.

The physical-chemical systems, which were investigated experimentally, were marked by round brackets. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. The designation "?" corresponds to the indeterminate result of predicring. According to our results the many new compounds with Al, Sc, Y, Fe, Co, Ni, Ga, and As have the crystal structure of hantite at normal pressure and room temperature. These compounds hold the promise for searching for new EO, nonlinear optical and laser materials.

Table 2.3.3.1

Table of Predictions of Crystal Structure Type for Compounds of Composition $AD(BO_3)_4$

D / A	Al	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Ga	As
Al	(-)	H	H	H	H	H	H	H	H	H	
Sc	H	(C)					H	H	H	H	
Ti	H	H	(C)				H	H		H	
V	H			(C)			H	H		H	
Cr	H				(C)		H	H		H	
Mn	H	H					H	H		H	
Fe	H						(C)	H		H	
Co	H	H			H	H	H			H	
Ni	H	H			H	H	H	H		H	
Ga	H	H					H	H	H	(C)	

D / A	Al	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Ga	As
As	H	H					H	H	H	H	
Y	(H)	H	H	H	(H)	H	(H)	H	H	(H)	H
Rh	H	H					H	H	H	H	
In	H	H					H	H	H	H	
Sb	H	H		H	H	H	H	H	H	H	
La	?	(-)	*	*	*	*	(H)	?	?	?	*
Ce	H	(H)	A	A	?	?	(H)	?	?	H	H
Pr	(H)	(H)			H	H	(H)	?	?	H	H
Nd	(H)	(H)	A	A	(H)	?	(H)	?	?	(H)	H
Pm			A	A	?	?	H	?	?	H	H
Sm	(H)	(H)	H	H	(H)	H	(H)	H	H	(H)	H
Eu	(H)	(H)					(H)	?	?	(H)	
Gd	(H)	H	H	H	(H)	H	(H)	H	H	(H)	
Tb	(H)	H			H	H	(H)	?	?	(H)	H
Dy	(H)	H			H	H	(H)	?	?	(H)	H
Ho	(H)				?	?	(H)	?	?	H	H
Er	(H)	H	H	H	H	H	H	H	H	H	
Tm	(H)						H	?	?	H	H
Yb	(H)	H		H	H	H	H	H	H	H	
Lu	(H)		?	A	?	?	H	?	?	H	?
Ir	H	?	C	C	?	?	H	?	?	H	

D / A	Al	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Ga	As
Tl					H	H	H	H	H	H	
Bi			H	H	H	H	H	H	H	H	
Ac	H	H			H	H	H	H	H	H	H
Pa	H	H	H	H	H	H	H	H	H	H	
U	H	H			H	H	H	H	H	H	
Np	H	H	H	H	H	H	H	H	H	H	
Pu			H	H	H	H	H	H	H	H	
Am			H	H	H	H	H	H	H	H	
Cm	H	H	H	H	H	H	H	H	H	H	
Bk	H	H	H	H	H	H	H	H	H	H	
Cf	H	H	H	H	H	H	H	H	H	H	

2.4. PREDICTION OF NEW COMPOUNDS OF COMPOSITION $A^{I}B^{II}C^{III}F_6$

Complicated fluorides with composition $ABCF_6$ are of great interest because they offer a potential basis for many applications (i.e., laser crystals (compounds $NaCaYF_6$, $NaCaCeF_6$, $NaCaErF_6$, colquirite ($LiCaAlF_6$)) [27,28], EO materials and materials for vacuum ultraviolet optics (limahalfite ($LiMgAlF_6$) and colquirite ($LiCaAlF_6$)) [2]).

Ravez mentions that compounds of composition $A^{I}Mn^{II}M^{III}F_6$ can have piezoelectric and nonlinear optical properties [30].

The most widespread for compounds $ABCF_6$ crystal structure types are: modified from pyrochlore structure ($RbNiCrF_6$) (space group Fd3m, Z=8), Na_2SiF_6 (space group P321, Z=3), trirutile (space group $P4_2/mnm$, Z= 2), colquirite (space group P3(-)1c, Z=2), and $CsAgFeF_6$ (space group Pnma, Z=4). Only compounds with crystal structure types Na_2SiF_6 and colquirite can have potentially EO, piezoelectric and nonlinear optical properties because they have acentric space groups.

Common features of Na_2SiF_6 and colquirite structures are quasi-hcp of anions and an occupancy of half the octahedral sites by cations. Differences arise from the type of sharing between MF_6 octahedra: in Na_2SiF_6, for instance, SiF_6 units share three edges with NaF_6 octahedra, whereas in $LiCaAlF_6$ only corners are shared betweeen LiF_6, CaF_6 and AlF_6 octahedra [31,32]. It is possible to consider Na_2SiF_6 and trirutile structures as different versions of colquirite structure [32]. The authors of [32] obtained the stability fields for colquirite, trirutile and Na_2SiF_6-structure types of compounds $LiB^{II}C^{III}F_6$. Trirutile structure forms if ratios r_{II}/r_{Li}, r_{III}/r_{Li}, and r_{II}/r_{III} lie within 0.9-1.2. Na_2SiF_6 structure forms if one or two ratios lie within 1.2-1.4. The colquirite structure forms for large B^{II} - cations if r_{II}/r_{Li} or r_{II}/r_{III} are more than 1.4.

It should be pointed out that compounds $A^{I}B^{II}C^{III}F_6$ are a result of heterovalent substitution of B^{IV}-ion in compounds $A^{I}B^{IV}F_6$. Previously we predicted the formation or non-formation of such compounds and

their crystal structure type at normal state [33] including Na_2SiF_6 - structure type. Solution of the problem of the computer design of multi-component compounds on the base of substitution of ions in more simple compounds allows to obtain the new substances with more interesting for practice properties than for an initial compound.

2.4.1. DATA FOR COMPUTER LEARNING

The data for computer learning was extracted from our the cardfile on quaternary inorganic compound properties. On the base of analysis of these data it may be concluded that only compounds $ABCF_6$ with A = Li and Na can crystallize in colquirite or Na_2SiF_6 structures. Therefore this structure at room state and normal pressure was predicted only for A = Li, Na and their analogs in Periodical Table: K, Rb and Cs. The table 2.4.1.1 contains a learning set.

Table 2.4.1.1

Learning Set for Prediction of the Crystal Structure Type of Compounds with Composition $ABCF_6$

Composition	Crystal type	Space group
LiMgAlF6	Na2SiF6	
LiMnAlF6	Na2SiF6	
LiMgInF6	Na2SiF6	
LiCaInF6	Na2SiF6	
LiMnTiF6	Na2SiF6	
LiMnVF6	Na2SiF6	
LiMnCrF6	Na2SiF6	
LiMnFeF6	Na2SiF6	
LiMnGaF6	Na2SiF6	
LiMnRhF6	Na2SiF6	
LiMnInF6	Na2SiF6	
LiFeGaF6	Na2SiF6	
LiCoInF6	Na2SiF6	
LiNiInF6	Na2SiF6	
LiZnInF6	Na2SiF6	
LiCdInF6	Na2SiF6	
NaMnAlF6	Na2SiF6	
NaCaAlF6	Na2SiF6	
NaMnCrF6	Na2SiF6	
NaMnFeF6	Na2SiF6	

Composition	Crystal type	Space group
LiMgTiF6	Trirutile	
LiMgVF6	Trirutile	
LiMgCrF6	Trirutile	
LiMgFeF6	Trirutile	
LiMgCoF6	Trirutile	
LiMgGaF6	Trirutile	
LiMgRhF6	Trirutile	
LiFeTiF6	Trirutile	
LiCoTiF6	Trirutile	
LiNiTiF6	Trirutile	
LiZnTiF6	Trirutile	
LiNiVF6	Trirutile	
LiZnVF6	Trirutile	
LiFeCrF6	Trirutile	
LiCoCrF6	Trirutile	
LiNiCrF6	Trirutile	
LiCuCrF6	Trirutile	
LiZnCrF6	Trirutile	
LiFeFeF6	Trirutile	
LiCoFeF6	Trirutile	
LiNiFeF6	Trirutile	
LiCuFeF6	Trirutile	
LiZnFeF6	Trirutile	
LiCoNiF6	Trirutile	
LiNiCoF6	Trirutile	
LiCuCoF6	Trirutile	
LiZnCoF6	Trirutile	
LiCoGaF6	Trirutile	
LiCoRhF6	Trirutile	
LiNiGaF6	Trirutile	
LiNiRhF6	Trirutile	
LiCuGaF6	Trirutile	
LiCuRhF6	Trirutile	
LiZnRhF6	Trirutile	
LiCaAlF6	LiCaAlF6	
LiSrAlF6	LiCaAlF6	
LiCaTiF6	LiCaAlF6	
LiCaVF6	LiCaAlF6	
LiCaCrF6	LiCaAlF6	
LiCaFeF6	LiCaAlF6	
LiCaCoF6	LiCaAlF6	
LiCaNiF6	LiCaAlF6	
LiCaGaF6	LiCaAlF6	

Composition	Crystal type	Space group
LiCaRhF6	LiCaAlF6	
LiSrTiF6	LiCaAlF6	
LiCdTiF6	LiCaAlF6	
LiSrVF6	LiCaAlF6	
LiCdVF6	LiCaAlF6	
LiPbVF6	LiCaAlF6	
LiSrCrF6	LiCaAlF6	
LiCdCrF6	LiCaAlF6	
LiPbCrF6	LiCaAlF6	
LiCdFeF6	LiCaAlF6	
LiPbFeF6	LiCaAlF6	
LiCdCoF6	LiCaAlF6	
LiSrNiF6	LiCaAlF6	
LiSrGaF6	LiCaAlF6	
LiPbGaF6	LiCaAlF6	
LiCdRhF6	LiCaAlF6	
RbMgAlF6	RbNiCrF6	
CsMgAlF6	RbNiCrF6	
CsMgTiF6	RbNiCrF6	
CsMgVF6	RbNiCrF6	
RbMgCrF6	RbNiCrF6	
CsMgCrF6	RbNiCrF6	
CsMgFeF6	RbNiCrF6	
RbMgCoF6	RbNiCrF6	
RbMgNiF6	RbNiCrF6	
CsMgNiF6	RbNiCrF6	
CsMgCuF6	RbNiCrF6	
CsMgGaF6	RbNiCrF6	
KNiAlF6	RbNiCrF6	
RbNiAlF6	RbNiCrF6	
CsNiAlF6	RbNiCrF6	
KNiCrF6	RbNiCrF6	
CsVScF6	RbNiCrF6	
CsPdScF6	RbNiCrF6	
CsAgScF6	RbNiCrF6	
CsCoTiF6	RbNiCrF6	
CsNiTiF6	RbNiCrF6	
CsCuTiF6	RbNiCrF6	
CsZnTiF6	RbNiCrF6	
CsVCrF6	RbNiCrF6	
CsVMnF6	RbNiCrF6	
RbVFeF6	RbNiCrF6	
CsVFeF6	RbNiCrF6	

Composition	Crystal type	Space group
CsCoVF6	RbNiCrF6	
CsNiVF6	RbNiCrF6	
CsCuVF6	RbNiCrF6	
CsZnVF6	RbNiCrF6	
RbMnCrF6	RbNiCrF6	
CsMnCrF6	RbNiCrF6	
RbFeCrF6	RbNiCrF6	
CsFeCrF6	RbNiCrF6	
RbCoCrF6	RbNiCrF6	
CsCoCrF6	RbNiCrF6	
RbNiCrF6	RbNiCrF6	
CsNiCrF6	RbNiCrF6	
RbCuCrF6	RbNiCrF6	
CsCuCrF6	RbNiCrF6	
RbZnCrF6	RbNiCrF6	
CsZnCrF6	RbNiCrF6	
CsMnFeF6	RbNiCrF6	
RbZnMnF6	RbNiCrF6	
CsZnMnF6	RbNiCrF6	
CsMnGaF6	RbNiCrF6	
CsCoFeF6	RbNiCrF6	
RbNiFeF6	RbNiCrF6	
CsNiFeF6	RbNiCrF6	
RbCuFeF6	RbNiCrF6	
CsCuFeF6	RbNiCrF6	
CsZnFeF6	RbNiCrF6	
CsPdFeF6	RbNiCrF6	
RbNiCoF6	RbNiCrF6	
RbCoNiF6	RbNiCrF6	
CsNiCoF6	RbNiCrF6	
CsCoNiF6	RbNiCrF6	
RbCuCoF6	RbNiCrF6	
RbZnCoF6	RbNiCrF6	
CsZnNiF6	RbNiCrF6	
CsNiGaF6	RbNiCrF6	
CsNiInF6	RbNiCrF6	
CsZnCuF6	RbNiCrF6	
CsCuGaF6	RbNiCrF6	
CsCuInF6	RbNiCrF6	
CsCuTlF6	RbNiCrF6	
CsZnInF6	RbNiCrF6	
CsPdRhF6	RbNiCrF6	
CsPdInF6	RbNiCrF6	

Composition	Crystal type	Space group
CsAgInF6	RbNiCrF6	
CsAgTlF6	RbNiCrF6	
RbCuAlF6	CsAgAlF6	
CsCuAlF6	CsAgAlF6	
CsZnAlF6	CsAgAlF6	
RbAgAlF6	CsAgAlF6	
CsAgAlF6	CsAgAlF6	
RbCuVF6	CsAgAlF6	
RbAgFeF6	CsAgAlF6	
CsAgFeF6	CsAgAlF6	
RbAgGaF6	CsAgAlF6	
CsAgGaF6	CsAgAlF6	
LiBaAlF6		P2(1)/c, Z=4
LiBaTiF6		P2(1)/c, Z=4
LiBaVF6		P2(1)/c, Z=4
LiBaCrF6		P2(1)/c, Z=4
LiBaFeF6		P2(1)/c, Z=4
LiBaCoF6		P2(1)/c, Z=4
LiBaGaF6		P2(1)/c, Z=4
KBeYF6		P2(1)/m, Z=2
KBeSmF6		P2(1)/m, Z=2
KBeEuF6		P2(1)/m, Z=2
KBeGdF6		P2(1)/m, Z=2
KBeTbF6		P2(1)/m, Z=2
KBeDyF6		P2(1)/m, Z=2
KBeHoF6		P2(1)/m, Z=2
KBeErF6		P2(1)/m, Z=2
KBeTmF6		P2(1)/m, Z=2
KBeYbF6		P2(1)/m, Z=2
KBeLuF6		P2(1)/m, Z=2
NaCaCeF6	UCl3	P6(3)/m, Z=1
NaBaCeF6	UCl3	P6(3)/m, Z=1
KCaCeF6	UCl3	P6(3)/m, Z=1
KCrMnF6	bronze	P4/mbm, Z=5
KCrFeF6	bronze	P4/mbm, Z=5
KCuCrF6		P2(1)/c, Z=4
KCoFeF6	bronze	P4/mbm, Z=5
KBaCeF6	UCl3	P6(3)/m, Z=1
RbMnFeF6	NH4MnFeF6	Pb2n
CsNiMnF6	CsNiMnF6	R3(-)m
KEuCeF6		P3(-), Z=1
LiF-BeF2-CeF3	without compound ABCF6	

Composition	Crystal type	Space group
KF-BeF2-LaF3	without compound ABCF6	
NaF-PbF2-BiF3	without compound ABCF6	
KF-CuF2-YbF3	without compound ABCF6	
KF-CuF2-LuF3	without compound ABCF6	
KF-CuF2-BiF3	without compound ABCF6	

2.4.2. SELECTION OF FEATURES

On the basis of physical-chemical grounds two sets of chemical elements features and set of simlpe fluorides feature were selected for the description of these systems.

2.4.2.1. FEATURE SET 2.4.1

The first feature set (feature set 2.4.1) includes information about the number of electrons in energy shells of isolated atoms and Shannon effective ionic radii of elements A (C.N.=6), B (C.N.=6) or C (C.N.=6) in the compound of composition $ABCF_6$. The grouping of energy shell information corresponds to the number of electrons for each shell. The quasi-continuous properties - the ionic radii - were divided using the special program of discretization [18]. Table 2.4.2.1.1 contains the gradations for Feature Set 2.4.1.

Table 2.4.2.1.1

Gradations for Feature Set 2.4.1

Feature	Gradation	Feature	Gradation
	A-element		
2s-shell		4d-shell	
s1	s2_1_1	d0	d4_0_1
s2	s2_2_1	d10	d4_10_1
2p-shell		5s-shell	
p0	p2_0_1	s0	s5_0_1
p6	p2_6_1	s1	s5_1_1
3s-shell		s2	s5_2_1
s0	s3_0_1	5p-shell	
s1	s3_1_1	p0	p5_0_1
s2	s3_2_1	p6	p5_6_1
3p-shell		6s-shell	
p0	p3_0_1	s0	s6_0_1

Feature	Gradation	Feature	Gradation
p6	p3_6_1	s1	s6_1_1
3d-shell		Ionic	
d0	d3_0_1	radius, A	
d10	d3_10_1	[0.76-0.7873]	R1_1
4s-shell		[1.0057-1.0421]	R2_1
s0	s4_0_1	[1.3697-1.4061]	R3_1
s1	s4_1_1	[1.4971-1.5426]	R4_1
s2	s4_2_1	[1.6518-1.67]	R5_1
4p-shell			
p0	p4_0_1		
p6	p4_6_1		
	B-element		
3s-shell		5s-shell	
s2	s3_2_2	s0	s5_0_2
3p-shell		s1	s5_1_2
p0	p3_0_2	s2	s5_2_2
p6	p3_6_2	5p-shell	
3d-shell		p0	p5_0_2
d0	d3_0_2	p6	p5_6_2
d2	d3_2_2	5d-shell	
d3	d3_3_2	d0	d5_0_2
d5	d3_5_2	d10	d5_10_2
d6	d3_6_2	6s-shell	
d7	d3_7_2	s0	s6_0_2
d8	d3_8_2	s2	s6_2_2
d10	d3_10_2	6p-shell	
4s-shell		p0	p6_0_2
s0	s4_0_2	p2	p6_2_2
s1	s4_1_2	Ionic	
s2	s4_2_2	radius, A	
4p-shell		[0.45-0.477]	R1_2
p0	p4_0_2	[0.675-0.765]	R2_2
p6	p4_6_2	(0.765-0.783]	R3_2
4d-shell		(0.783-0.792]	R4_2
d0	d4_0_2	(0.792-0.819]	R5_2
d10	d4_10_2	(0.819-0.855]	R6_2
4f-shell		(0.855-0.882]	R7_2
f0	f4_0_2	[0.918-0.945]	R8_2
f14	f4_14_2	(0.945-0.972]	R9_2
		[0.99-1.026]	R10_2
		[1.152-1.179]	R11_2
		(1.179-1.188]	R12_2

Feature	Gradation	Feature	Gradation
		(1.188-1.215]	R13_2
		[1.323-1.35]	R14_2
	C-element		
3p-shell		5p-shell	
p1	p3_1_3	p0	p5_0_3
p6	p3_6_3	p1	p5_1_3
3d-shell		p6	p5_6_3
d0	d3_0_3	5d-shell	
d1	d3_1_3	d0	d5_0_3
d2	d3_2_3	d10	d5_10_3
d3	d3_3_3	6s-shell	
d5	d3_5_3	s0	s6_0_3
d6	d3_6_3	s2	s6_2_3
d7	d3_7_3	6p-shell	
d8	d3_8_3	p0	p6_0_3
d10	d3_10_3	p1	p6_1_3
4s-shell		Ionic	
s0	s4_0_3	radius, A	
s1	s4_1_3	[0.27-0.53997]	R1_3
s2	s4_2_3	(0.53997-0.55488]	R2_3
4p-shell		[0.58-0.60955]	R3_3
p0	p4_0_3	(0.60955-0.61452]	R4_3
p1	p4_1_3	(0.61452-0.61949]	R5_3
p3	p4_3_3	(0.61949-0.64434]	R6_3
p6	p4_6_3	(0.64434-0.65925]	R7_3
4d-shell		(0.65925-0.66919]	R8_3
d0	d4_0_3	(0.66919-0.6841]	R9_3
d1	d4_1_3	[0.69-0.75865]	R10_3
d8	d4_8_3	[0.76-0.81332]	R11_3
d10	d4_10_3	[0.85-0.87793]	R12_3
4f-shell		(0.87793-0.8829]	R13_3
f0	f4_0_3	(0.8829-0.88787]	R14_3
f14	f4_14_3	(0.88787-0.97236]	R15_3
5s-shell		[0.975-1.02206]	R16_3
s0	s5_0_3	(1.02206-1.12]	R17_3
s1	s5_1_3		
s2	s5_2_3		

2.4.2.2. FEATURE SET 2.4.2

The second feature set (feature set 2.4.2) includes the following in-

formation: the first three ionization potentials, the electronegativities by Pauling, the entropies of the individual substances at 298 K, the isobaric thermal capacities at 298 K, the temperatures and the heats of melting and boiling, Debye temperatures, the energies of the crystal lattice, the ionic radii by Shannon, the ratio of the atomic number to the average atomic mass for atoms of elements A, B and C. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.4.2.2.1 contains the gradations for Feature Set 2.4.2.

Table 2.4.2.2.1

Gradations for Feature Set 2.4.2

Feature	Gradation	Feature	Gradation
	A-element		
First ionization potential, eV		Boiling point, K	
[3.89391-3.938847]	I1_1_1	[945-978.4]	Tb_1_1
[4.148551-4.208467]	I1_2_1	[1018.48-1051.88]	Tb_2_1
[4.29834-4.373235]	I1_3_1	[1145.4-1178.8]	Tb_3_1
[5.12218-5.182096]	I1_4_1	[1592.96-1613]	Tb_4_1
[5.361842-5.3918]	I1_5_1	Heat of melting, kJ/mol	
Second ionization potential, eV		[2.096-2.24816]	Hm_1_1
[23.1575-24.732]	I2_1_1	[2.29888-2.40032]	Hm_2_1
[25.78167-28.40585]	I2_2_1	[2.55248-2.65392]	Hm_3_1
[30.50519-33.12936]	I2_3_1	[4.58128-4.632]	Hm_4_1
[45.7254-48.34958]	I2_4_1	Heat of boiling, kJ/mol	
[74.59133-75.641]	I2_5_1	[76.442-78.2909]	Hb_1_1
Third ionization potential, eV		[79.5235-81.9887]	Hb_2_1
[33.4-36.0715]	I3_1_1	[86.91911-90.0006]	Hb_3_1
[37.8525-41.4145]	I3_2_1	[106.0244-108.4896]	Hb_4_1
[43.1955-47.648]	I3_3_1	[136.8394-138.072]	Hb_5_1
[69.02-73.4725]	I3_4_1	Energy of the crystal lattice, -6 E*10 J/kg*mol	
[119.7785-122.45]	I3_5_1		
Electronegativity			
[0.7-0.709]	X_1_1	[79-81.286]	E_1_1
[0.793-0.808]	X_2_1	[84.334-88.144]	E_2_1
[0.892-0.907]	X_3_1	(88.144-91.954]	E_3_1
[0.991-1]	X_4_1	[107.194-111.004]	E_4_1
Entropies of individual substances at 298 K kJ/kg*mol*K		[153.676-155.2]	E_5_1
		Debye temperature, K	
[29.121-30.80421]	S_1_1	[39.2-62.356]	Td_1_1
		[82.204-98.744]	Td_2_1

Feature	Gradation	Feature	Gradation
[49.88059-52.68594]	S_2_1	[151.672-168.212]	Td_3_1
[63.90734-66.15162]	S_3_1	[360.076-370]	Td_4_1
[75.12874-77.93409]	S_4_1	Ratio of the	
[83.54478-85.228]	S_5_1	atomic number	
Isobaric thermal		to the average	
capacity at 298 K,		atomic mass	
kJ/kg*mol*K		[0.41-0.4124]	NM_1_1
[24.853-25.07266]	Cp_1_1	[0.4284-0.4316]	NM_2_1
[28.00146-28.36756]	Cp_2_1	[0.478-0.482]	NM_3_1
[29.39264-29.68552]	Cp_3_1	[0.4884-0.49]	NM_4_1
[30.85704-31.22314]	Cp_4_1	Ionic radius, A	
[31.95534-32.175]	Cp_5_1	[0.76-0.7873]	Rs_1_1
Melting point, K		[1.0057-1.0421]	Rs_2_1
[301.67-306.2309]	Tm_1_1	[1.3697-1.4061]	Rs_3_1
[309.2715-316.873]	Tm_2_1	[1.4971-1.5426]	Rs_4_1
[335.1166-341.1978]	Tm_3_1	[1.6518-1.67]	Rs_5_1
[368.5632-374.6444]	Tm_4_1		
[450.6594-453.7]	Tm_5_1		
	B-element		
First ionization		Boiling point, K	
potential, eV		[630-1118.86]	Tb_1_2
[5.21166-5.337139]	I1_1_2	(1118.86-1250.878]	Tb_2_2
[5.588098-5.671751]	I1_2_2	[1303.685-1435.703]	Tb_3_2
(5.671751-5.79723]	I1_3_2	[1593-1699.738]	Tb_4_2
[6.048188-6.215494]	I1_4_2	(1699.738-1752.545]	Tb_5_2
[6.254-6.759237]	I1_5_2	(1752.545-1831.755]	Tb_6_2
(6.759237-6.884716]	I1_6_2	[1990.176-2095.79]	Tb_7_2
[7.30298-7.428459]	I1_7_2	(2095.79-2201.404]	Tb_8_2
(7.428459-7.553938]	I1_8_2	[2307.018-2412.632]	Tb_9_2
(7.553938-7.595765]	I1_9_2	(2412.632-2491.843]	Tb_10_2
(7.595765-7.846724]	I1_10_2	[2703.071-2808.685]	Tb_11_2
(7.846724-8.014029]	I1_11_2	(2808.685-2887.895]	Tb_12_2
[8.264987-8.432293]	I1_12_2	(2887.895-2940.702]	Tb_13_2
[8.93421-9.101516]	I1_13_2	(2940.702-3019.913]	Tb_14_2
[9.268821-9.352474]	I1_14_2	[3072.719-3151.93]	Tb_15_2
(9.352474-10.4376]	I1_15_2	(3151.93-3204.737]	Tb_16_2
Second ionization		(3204.737-3283.948]	Tb_17_2
potential, eV		[3600-4100]	Tb_18_2
[10.004-10.34858]	I2_1_2	Heat of melting,	
[10.80802-11.1526]	I2_2_2	kJ/mol	
(11.1526-11.49718]	I2_3_2	[2.295-5.324186]	Hm_1_2
[11.7269-12.18634]	I2_4_2	[5.688883-6.600626]	Hm_2_2

Feature	Gradation	Feature	Gradation
[13.57-14.94298]	I2_5_2	(6.600626-7.147672]	Hm_3_2
(14.94298-15.28756]	I2_6_2	(7.147672-7.694717]	Hm_4_2
[15.51728-15.97672]	I2_7_2	[8.059415-8.424112]	Hm_5_2
(15.97672-16.43616]	I2_8_2	(8.424112-8.971158]	Hm_6_2
(16.43616-16.78074]	I2_9_2	[9.21096-10.97699]	Hm_7_2
(16.78074-17.01046]	I2_10_2	(10.97699-11.70639]	Hm_8_2
(17.01046-17.35504]	I2_11_2	(11.70639-12.43578]	Hm_9_2
[17.81448-18.50364]	I2_12_2	(12.43578-12.80048]	Hm_10_2
[18.56-19.7671]	I2_13_2	(12.80048-13.34752]	Hm_11_2
[19.99682-20.57112]	I2_14_2	(13.34752-14.25927]	Hm_12_2
[21.26028-21.49]	I2_15_2	[15.061-16.6298]	Hm_13_2
Third ionization		(16.6298-17.17684]	Hm_14_2
potential, eV		(17.17684-17.90624]	Hm_15_2
[24.9-28.77]	I3_1_2	[19.665-21.37086]	Hm_16_2
(28.77-30.06]	I3_2_2	[22.46495-31.81968]	Hm_17_2
(30.06-31.35]	I3_3_2	Heat of boiling,	
(31.35-32.64]	I3_4_2	kJ/mol	
(32.64-33.93]	I3_5_2	[59.229-109.9344]	Hb_1_2
(33.93-35.22]	I3_6_2	(109.9344-123.7416]	Hb_2_2
(35.22-41.67]	I3_7_2	[137.5488-151.356]	Hb_3_2
(41.67-45.54]	I3_8_2	(151.356-161.7114]	Hb_4_2
[48.12-54.57]	I3_9_2	(161.7114-175.5186]	Hb_5_2
[77.79-82.95]	I3_10_2	(175.5186-182.4222]	Hb_6_2
[150.03-153.9]	I3_11_2	(182.4222-192.7776]	Hb_7_2
Electronegativity		[220.392-234.1992]	Hb_8_2
[0.9-0.939]	X_1_2	[241.1028-258.3618]	Hb_9_2
[0.965-1.03]	X_2_2	[292.8798-310.1388]	Hb_10_2
[1.082-1.134]	X_3_2	(310.1388-323.946]	Hb_11_2
[1.186-1.238]	X_4_2	[330.8496-348.1086]	Hb_12_2
[1.472-1.537]	X_5_2	(348.1086-351.5604]	Hb_13_2
[1.563-1.628]	X_6_2	(351.5604-361.9158]	Hb_14_2
[1.68-1.732]	X_7_2	(361.9158-372.2712]	Hb_15_2
[1.784-1.836]	X_8_2	(372.2712-382.6266]	Hb_16_2
[1.862-1.927]	X_9_2	[410.44-510.448]	Hb_17_2
[2.161-2.2]	X_10_2	Energy of the	
Entropies of		crystal lattice,	
individual		-6	
substances at 298 K		E*10 J/kg*mol	
kJ/kg*mol*K		[116-127.61]	E_1_2
[9.498-11.34833]	S_1_2	(127.61-158.57]	E_2_2
[22.4503-24.9174]	S_2_2	(158.57-174.05]	E_3_2
[26.15095-28.61806]	S_3_2	(174.05-185.66]	E_4_2
(28.61806-29.85161]	S_4_2	(185.66-205.01]	E_5_2

Feature	Gradation	Feature	Gradation
(29.85161-31.70193]	S_5_2	[274.67-286.28]	E_6_2
(31.70193-32.31871]	S_6_2	(286.28-297.89]	E_7_2
(32.31871-34.78582]	S_7_2	[313.37-332.72]	E_8_2
[36.01937-39.10325]	S_8_2	(332.72-340.46]	E_9_2
[40.3368-42.18713]	S_9_2	(340.46-352.07]	E_10_2
(42.18713-44.03746]	S_10_2	[359.81-375.29]	E_11_2
[50.20522-53.2891]	S_11_2	[383.03-398.51]	E_12_2
[54.52265-57.60653]	S_12_2	(398.51-413.99]	E_13_2
[61.30718-63.77429]	S_13_2	[421.73-429.47]	E_14_2
[66.24139-69.32527]	S_14_2	(429.47-441.08]	E_15_2
(69.32527-79.898]	S_15_2	[470-510]	E_16_2
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		Debye temperature, K	
[16.443-16.79196]	Cp_1_2	[75-126.95]	Td_1_2
[23.07324-23.65484]	Cp_2_2	(126.95-158.9]	Td_2_2
[24.12012-24.70172]	Cp_3_2	(158.9-222.8]	Td_3_2
(24.70172-24.81804]	Cp_4_2	(222.8-254.75]	Td_4_2
(24.81804-24.93436]	Cp_5_2	(254.75-297.35]	Td_5_2
(24.93436-25.28332]	Cp_6_2	(297.35-371.9]	Td_6_2
(25.28332-25.39964]	Cp_7_2	(371.9-403.85]	Td_7_2
(25.39964-25.7486]	Cp_8_2	(403.85-435.8]	Td_8_2
(25.7486-25.86492]	Cp_9_2	(435.8-446.45]	Td_9_2
(25.86492-25.98124]	Cp_10_2	(446.45-457.1]	Td_10_2
(25.98124-26.21388]	Cp_11_2	[465-489.05]	Td_11_2
(26.21388-26.3302]	Cp_12_2	[574.25-616.85]	Td_12_2
(26.3302-26.67916]	Cp_13_2	[1128.05-1160]	Td_13_2
(26.67916-26.79548]	Cp_14_2	Ratio of the atomic number to the average atomic mass	
(26.79548-27.14444]	Cp_15_2		
[27.84236-28.075]	Cp_16_2		
Melting point, K		[0.4-0.403]	NM_1_2
[234-641.88]	Tm_1_2	[0.407-0.412]	NM_2_2
[673.8-737.64]	Tm_2_2	[0.428-0.432]	NM_3_2
[897.24-961.08]	Tm_3_2	[0.438-0.442]	NM_4_2
(961.08-1040.88]	Tm_4_2	[0.448-0.452]	NM_5_2
(1040.88-1088.76]	Tm_5_2	[0.458-0.462]	NM_6_2
(1088.76-1104.72]	Tm_6_2	[0.468-0.472]	NM_7_2
(1104.72-1152.6]	Tm_7_2	[0.478-0.482]	NM_8_2
[1210.4-1280.28]	Tm_8_2	[0.488-0.492]	NM_9_2
[1312.2-1392]	Tm_9_2	[0.498-0.5]	NM_10_2
[1519.68-1599.48]	Tm_10_2	Ionic radius, A	
[1695.24-1759.08]	Tm_11_2	[0.45-0.477]	Rs_1_2
(1759.08-1822.92]	Tm_12_2	[0.675-0.765]	Rs_2_2

Feature	Gradation	Feature	Gradation
(1822.92-1941]	Tm_13_2	(0.765-0.783]	Rs_3_2
[2045-2174.04]	Tm_14_2	(0.783-0.792]	Rs_4_2
(2174.04-2190]	Tm_15_2	(0.792-0.819]	Rs_5_2
		(0.819-0.855]	Rs_6_2
		(0.855-0.882]	Rs_7_2
		[0.918-0.945]	Rs_8_2
		(0.945-0.972]	Rs_9_2
		[0.99-1.026]	Rs_10_2
		[1.152-1.179]	Rs_11_2
		(1.179-1.188]	Rs_12_2
		(1.188-1.215]	Rs_13_2
		[1.323-1.35]	Rs_14_2
	C-element		
First ionization potential, eV		Boiling point, K	
[5.2-5.500292]	I1_1_3	[885-1657.5]	Tb_1_3
(5.500292-5.574584]	I1_2_3	(1657.5-1743.5]	Tb_2_3
(5.574584-5.624112]	I1_3_3	(1743.5-1808]	Tb_3_3
(5.624112-5.723168]	I1_4_3	(1808-1872.5]	Tb_4_3
(5.723168-5.846988]	I1_5_3	[1906-2044.5]	Tb_5_3
(5.846988-5.970808]	I1_6_3	[2259.5-2345.5]	Tb_6_3
(5.970808-6.020336]	I1_7_3	(2345.5-2410]	Tb_7_3
(6.020336-6.094628]	I1_8_3	[2432-2539]	Tb_8_3
(6.094628-6.144156]	I1_9_3	(2539-2775.5]	Tb_9_3
(6.144156-6.243212]	I1_10_3	(2775.5-2797]	Tb_10_3
(6.243212-6.317504]	I1_11_3	(2797-2861.5]	Tb_11_3
[6.515616-6.614672]	I1_12_3	(2861.5-3012]	Tb_12_3
[6.713728-6.763256]	I1_13_3	(3012-3119.5]	Tb_13_3
(6.763256-6.812784]	I1_14_3	(3119.5-3227]	Tb_14_3
(6.812784-6.887076]	I1_15_3	(3227-3384]	Tb_15_3
[7.0923-7.357592]	I1_16_3	[3472-3635.5]	Tb_16_3
[7.365-7.456648]	I1_17_3	(3635.5-3678.5]	Tb_17_3
(7.456648-7.53094]	I1_18_3	(3678.5-5770]	Tb_18_3
[7.5762-7.704288]	I1_19_3	Heat of melting, kJ/mol	
(7.704288-7.77858]	I1_20_3	[2.8-3.85644]	Hm_1_3
[7.828108-7.877636]	I1_21_3	(3.85644-4.84384]	Hm_2_3
(7.877636-9.789]	I1_22_3	[5.2388-6.02872]	Hm_3_3
Second ionization potential, eV		[8.79344-9.78084]	Hm_4_3
		[10.04831-10.57076]	Hm_5_3
[10.6-11.09145]	I2_1_3	(10.57076-11.1632]	Hm_6_3
(11.09145-11.1886]	I2_2_3	(11.1632-11.75564]	Hm_7_3
(11.1886-12.1601]	I2_3_3	(11.75564-12.54556]	Hm_8_3

Feature	Gradation	Feature	Gradation
(12.1601-12.45155]	I2_4_3	(12.54556-13.53296]	Hm_9_3
[12.64585-13.03445]	I2_5_3	(13.53296-14.4]	Hm_10_3
[13.42305-14.1031]	I2_6_3	[14.6537-15.31028]	Hm_11_3
[14.31-14.8803]	I2_7_3	(15.31028-15.90272]	Hm_12_3
[15.4632-15.8518]	I2_8_3	(15.90272-16.29768]	Hm_13_3
[16.0461-16.629]	I2_9_3	(16.29768-16.89012]	Hm_14_3
(16.629-16.92045]	I2_10_3	(16.89012-17.48256]	Hm_15_3
(16.92045-17.30905]	I2_11_3	(17.48256-18.075]	Hm_16_3
[17.89195-18.08625]	I2_12_3	(18.075-18.86492]	Hm_17_3
(18.08625-18.3777]	I2_13_3	(18.86492-19.65484]	Hm_18_3
[18.572-18.86345]	I2_14_3	[20.084-21.43216]	Hm_19_3
(18.86345-19.1549]	I2_15_3	(21.43216-22.0246]	Hm_20_3
[19.42-20.41785]	I2_16_3	[22.41956-52]	Hm_21_3
(20.41785-25.155]	I2_17_3	Heat of boiling, kJ/mol	
Third ionization potential, eV		[31.798-180.6053]	Hb_1_3
[19.18-19.7098]	I3_1_3	(180.6053-190.4552]	Hb_2_3
(19.7098-20.4162]	I3_2_3	[203.5885-223.2884]	Hb_3_3
(20.4162-20.946]	I3_3_3	(223.2884-236.4217]	Hb_4_3
(20.946-21.4758]	I3_4_3	(236.4217-249.555]	Hb_5_3
(21.4758-24.1248]	I3_5_3	(249.555-262.6883]	Hb_6_3
[24.478-24.8312]	I3_6_3	[288.9548-295.5215]	Hb_7_3
(24.8312-25.0078]	I3_7_3	(295.5215-298.8048]	Hb_8_3
(25.0078-25.5376]	I3_8_3	(298.8048-308.6548]	Hb_9_3
(25.5376-26.0674]	I3_9_3	(308.6548-318.5047]	Hb_10_3
[27-27.8334]	I3_10_3	(318.5047-330.954]	Hb_11_3
(27.8334-28.3632]	I3_11_3	[334.9213-357.9046]	Hb_12_3
(28.3632-29.776]	I3_12_3	[364.4712-374.3212]	Hb_13_3
(29.776-30.3058]	I3_13_3	(374.3212-385.186]	Hb_14_3
(30.3058-30.659]	I3_14_3	[403.871-417.0043]	Hb_15_3
(30.659-30.8356]	I3_15_3	(417.0043-426.8543]	Hb_16_3
(30.8356-31.0122]	I3_16_3	[439.9875-453.1208]	Hb_17_3
(31.0122-31.542]	I3_17_3	[460.547-744.752]	Hb_18_3
[32.8-34.191]	I3_18_3	Energy of the crystal lattice, $E*10^{-6}$ J/kg*mol	
[34.7-35.7804]	I3_19_3		
[36.4868-37.931]	I3_20_3		
Electronegativity			
[1.1-1.133]	X_1_3	[182.8-194.671]	E_1_3
[1.177-1.232]	X_2_3	[202.585-218.413]	E_2_3
[1.276-1.331]	X_3_3	[234.241-254.4]	E_3_3
[1.485-1.529]	X_4_3	[269.854-297.553]	E_4_3
[1.573-1.628]	X_5_3	[305.467-325.252]	E_5_3
[1.672-1.727]	X_6_3	[333.166-341.08]	E_6_3

Feature	Gradation	Feature	Gradation
[1.771-1.826]	X_7_3	(341.08-352.951]	E_7_3
[1.87-1.925]	X_8_3	(352.951-368.779]	E_8_3
[2.167-2.4]	X_9_3	(368.779-380.65]	E_9_3
Entropies of individual substances at 298 K kJ/kg*mol*K		(380.65-400.435]	E_10_3
		(400.435-428.134]	E_11_3
		(428.134-440.005]	E_12_3
		[463.747-479.575]	E_13_3
[5.853-25.17534]	S_1_3	[495.403-524]	E_14_3
[26.19891-28.24603]	S_2_3	[566.629-775]	E_15_3
(28.24603-29.78137]	S_3_3	Debye temperature, K	
(29.78137-30.29316]	S_4_3		
(30.29316-31.31672]	S_5_3	[89-93.96]	Td_1_3
(31.31672-31.8285]	S_6_3	(93.96-108.84]	Td_2_3
(31.8285-32.85206]	S_7_3	(108.84-113.8]	Td_3_3
(32.85206-34.38741]	S_8_3	(113.8-118.76]	Td_4_3
[35.47-38.99343]	S_9_3	(118.76-128.68]	Td_5_3
[40.017-42.5759]	S_10_3	(128.68-143.56]	Td_6_3
[44.62303-47.405]	S_11_3	(143.56-163.4]	Td_7_3
[48.2055-50.25262]	S_12_3	(163.4-178.28]	Td_8_3
[50.3671-57.41756]	S_13_3	[199-232.84]	Td_9_3
(57.41756-58.9529]	S_14_3	[244-341.96]	Td_10_3
[62.02359-64.07072]	S_15_3	(341.96-356.84]	Td_11_3
(64.07072-65.60606]	S_16_3	[366.76-391.56]	Td_12_3
(65.60606-69.18853]	S_17_3	[411.4-441.16]	Td_13_3
(69.18853-70.72387]	S_18_3	(441.16-461]	Td_14_3
(70.72387-74.81812]	S_19_3	(461-475.88]	Td_15_3
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		(475.88-490.76]	Td_16_3
		[570.12-1219]	Td_17_3
[11.088-21.25769]	Cp_1_3	Ratio of the atomic number to the average atomic mass	
[23.14443-23.77335]	Cp_2_3		
[24.057-24.40227]	Cp_3_3		
(24.40227-24.71672]	Cp_4_3	[0.39-0.4024]	NM_1_3
(24.71672-24.87395]	Cp_5_3	[0.4088-0.412]	NM_2_3
(24.87395-25.50287]	Cp_6_3	[0.42-0.432]	NM_3_3
[25.81733-26.13179]	Cp_7_3	[0.4384-0.4416]	NM_4_3
(26.13179-26.28901]	Cp_8_3	[0.448-0.452]	NM_5_3
(26.28901-26.60347]	Cp_9_3	[0.4584-0.4624]	NM_6_3
(26.60347-26.7607]	Cp_10_3	[0.4688-0.472]	NM_7_3
(26.7607-26.91793]	Cp_11_3	[0.4784-0.48]	NM_8_3
(26.91793-27.23239]	Cp_12_3	Ionic radius, A	
(27.23239-27.70407]	Cp_13_3	[0.27-0.53997]	Rs_1_3
(27.70407-28.01853]	Cp_14_3	(0.53997-0.55488]	Rs_2_3

Feature	Gradation	Feature	Gradation
(28.01853-28.64745]	Cp_15_3	[0.57-0.60955]	Rs_3_3
[29.45-36.5089]	Cp_16_3	(0.60955-0.61452]	Rs_4_3
Melting point, K		(0.61452-0.61949]	Rs_5_3
[303-360.99]	Tm_1_3	(0.61949-0.64434]	Rs_6_3
[399.65-476.97]	Tm_2_3	(0.64434-0.65925]	Rs_7_3
[515.63-573.62]	Tm_3_3	(0.65925-0.66919]	Rs_8_3
(573.62-631.61]	Tm_4_3	(0.66919-0.6841]	Rs_9_3
[902.23-979.55]	Tm_5_3	[0.69-0.75865]	Rs_10_3
[1056.87-1095.53]	Tm_6_3	[0.76-0.81332]	Rs_11_3
(1095.53-1153.52]	Tm_7_3	[0.84-0.87793]	Rs_12_3
(1153.52-1250.17]	Tm_8_3	(0.87793-0.8829]	Rs_13_3
[1288.83-1346.82]	Tm_9_3	(0.8829-0.88787]	Rs_14_3
(1346.82-1406]	Tm_10_3	(0.88787-0.975]	Rs_15_3
[1499-1578.78]	Tm_11_3	[0.982-1.02206]	Rs_16_3
(1578.78-1714.09]	Tm_12_3	(1.02206-1.12]	Rs_17_3
(1714.09-1733.42]	Tm_13_3		
(1733.42-1752.75]	Tm_14_3		
(1752.75-1772.08]	Tm_15_3		
(1772.08-1810.74]	Tm_16_3		
(1810.74-1868.73]	Tm_17_3		
[1907.39-1984.71]	Tm_18_3		
[2139.35-2178.01]	Tm_19_3		
(2178.01-2216.67]	Tm_20_3		
(2216.67-3287]	Tm_21_3		

2.4.2.3. FEATURE SET 2.4.3

The third set of properties of simple fluorides (feature set 2.4.3) includes the following information of simple fluorides AF_2, BF_3 and CF_4 : the melting point, standard enthalpy of formation, standard isobaric thermal capacities, standard entropies, effective ionic radii of correspoding cations by Shannon. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.4.2.3.1 contains the gradations for Feature Set 2.4.3.

Table 2.4.2.3.1

Gradations for Feature Set 2.4.3
(Properties of Simple Fluorides)

Feature	Gradation	Feature	Gradation
	AF		
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[78-80.0673]	H_1_1	[9.99-10.0833]	Cp_1_1
[131.0607-134.5062]	H_2_1	[11.1407-11.2651]	Cp_2_1
(134.5062-136.5735]	H_3_1	[11.6383-11.7938]	Cp_3_1
(136.5735-138.6408]	H_4_1	[12.0426-12.167]	Cp_4_1
[145.5318-146.91]	H_5_1	(12.167-12.2914]	Cp_5_1
Standard entropy for corresponding simple fluorides, cal/mol*K		[13.0378-13.1]	Cp_6_1
		Melting point of simple fluorides, K	
		[600-620.04]	Tm_1_1
		[967.4-994.12]	Tm_2_1
[8.523-8.95341]	So_1_1	[1034.2-1067.6]	Tm_3_1
[11.82281-12.54016]	So_2_1	[1107.68-1127.72]	Tm_4_1
[15.6965-16.27038]	So_3_1	(1127.72-1147.76]	Tm_5_1
[18.27896-18.99631]	So_4_1	[1254.64-1268]	Tm_6_1
[21.86571-22.58306]	So_5_1	Ionic radii, A	
(22.58306-22.87]	So_6_1	[0.76-0.7873]	Rs_1_1
		[1.0057-1.0421]	Rs_2_1
		[1.3697-1.4061]	Rs_3_1
		[1.4789-1.5153]	Rs_4_1
		(1.5153-1.5426]	Rs_5_1
		[1.6518-1.67]	Rs_6_1
	BF 2		
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[82-95]	H_1_2	[12.39-12.5493]	Cp_1_2
[108.549-116.785]	H_2_2	[14.1423-14.3547]	Cp_2_2
[125.021-140]	H_3_2	[14.5671-14.8326]	Cp_3_2
[153.847-157.965]	H_4_2	[15.1512-15.4167]	Cp_4_2
(157.965-160.024]	H_5_2	[15.6291-15.8415]	Cp_5_2
(160.024-172.378]	H_6_2	[15.9477-16.1601]	Cp_6_2
		(16.1601-16.2663]	Cp_7_2

Feature	Gradation	Feature	Gradation
[180.614-184.732]	H_7_2	(16.2663-16.5849]	Cp_8_2
(184.732-190.909]	H_8_2	(16.5849-16.7973]	Cp_9_2
[195.027-201.204]	H_9_2	(16.7973-16.9566]	Cp_10_2
(201.204-207.381]	H_10_2	(16.9566-17.1159]	Cp_11_2
[240.325-250.62]	H_11_2	[17.5407-17.7]	Cp_12_2
[262.974-273.269]	H_12_2	Melting point of	
[281.505-289.741]	H_13_2	simple fluorides, K	
(289.741-291.8]	H_14_2	[385-991.63]	Tm_1_2
Standard entropy		[1034.89-1063.73]	Tm_2_2
for corresponding		(1063.73-1085.36]	Tm_3_2
simple fluorides,		(1085.36-1114.2]	Tm_4_2
cal/mol*K		(1114.2-1143.04]	Tm_5_2
[12.75-13.1775]	So_1_2	(1143.04-1164.67]	Tm_6_2
[13.4625-14.0325]	So_2_2	(1164.67-1186.3]	Tm_7_2
[16.0275-16.74]	So_3_2	[1215.14-1250]	Tm_8_2
[17.31-18.0225]	So_4_2	[1330.5-1366.55]	Tm_9_2
[18.8775-19.4475]	So_5_2	(1366.55-1417.02]	Tm_10_2
(19.4475-19.59]	So_6_2	(1417.02-1445.86]	Tm_11_2
(19.59-19.875]	So_7_2	[1517.96-1554.01]	Tm_12_2
(19.875-20.3025]	So_8_2	[1582.85-1597.27]	Tm_13_2
(20.3025-21.1575]	So_9_2	(1597.27-1618.9]	Tm_14_2
[22.0125-22.44]	So_10_2	[1662.16-1683.79]	Tm_15_2
(22.44-22.8675]	So_11_2	(1683.79-1691]	Tm_16_2
(22.8675-24]	So_12_2	Ionic radii, A	
[26.5-27]	So_13_2	[0.45-0.477]	Rs_1_2
		[0.675-0.765]	Rs_2_2
		(0.765-0.783]	Rs_3_2
		(0.783-0.792]	Rs_4_2
		(0.792-0.819]	Rs_5_2
		(0.819-0.855]	Rs_6_2
		(0.855-0.882]	Rs_7_2
		[0.918-0.945]	Rs_8_2
		(0.945-0.972]	Rs_9_2
		[0.99-1.026]	Rs_10_2
		[1.17-1.188]	Rs_11_2
		(1.188-1.215]	Rs_12_2
		[1.323-1.355]	Rs_13_2

Feature	Gradation	Feature	Gradation
	CF 3		
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[103.1-194.128]	H_1_3	[8.22-8.622001]	Cp_1_3
[213.256-222.82]	H_2_3	[17.734-18.27]	Cp_2_3
[228.7-244.339]	H_3_3	[18.538-19.208]	Cp_3_3
(244.339-253.903]	H_4_3	[21.352-30.25]	Cp_4_3
(253.903-261.076]	H_5_3	Melting point of simple fluorides, K	
[265.858-282.595]	H_6_3	[267-853.06]	Tm_1_3
[339.979-349.543]	H_7_3	[973.3-1023.4]	Tm_2_3
[354.325-366.28]	H_8_3	[1203.76-1253.86]	Tm_3_3
[374.3-392.581]	H_9_3	[1273.9-1374.1]	Tm_4_3
(392.581-394.972]	H_10_3	[1394.14-1434.22]	Tm_5_3
(394.972-406.927]	H_11_3	(1434.22-1444.24]	Tm_6_3
(406.927-411.709]	H_12_3	(1444.24-1454.26]	Tm_7_3
(411.709-414.1]	H_13_3	(1454.26-1484.32]	Tm_8_3
Standard entropy for corresponding simple fluorides, cal/mol*K		(1484.32-1504.36]	Tm_9_3
		(1504.36-1534.42]	Tm_10_3
		(1534.42-1574.5]	Tm_11_3
		(1574.5-1604.56]	Tm_12_3
[15.89-17.1629]	So_1_3	[1650-1704.76]	Tm_13_3
(17.1629-18.8601]	So_2_3	(1704.76-1734.82]	Tm_14_3
[20.5573-22.2545]	So_3_3	[1750-1794.94]	Tm_15_3
(22.2545-23.9517]	So_4_3	(1794.94-1825]	Tm_16_3
(23.9517-24.8003]	So_5_3	Ionic radii, A	
(24.8003-25.6489]	So_6_3	[0.27-0.54991]	Rs_1_3
(25.6489-26.4975]	So_7_3	[0.58-0.61452]	Rs_2_3
(26.4975-27.3461]	So_8_3	(0.61452-0.61949]	Rs_3_3
(27.3461-27.7704]	So_9_3	(0.61949-0.6344]	Rs_4_3
(27.7704-28.1947]	So_10_3	(0.6344-0.65925]	Rs_5_3
(28.1947-29.8919]	So_11_3	(0.65925-0.66919]	Rs_6_3
[30.14-33.7106]	So_12_3	(0.66919-0.6841]	Rs_7_3
(33.7106-43.3]	So_13_3	[0.72-0.76]	Rs_8_3
[57.0471-60.7]	So_14_3	[0.78847-0.81332]	Rs_9_3
		[0.85-0.87793]	Rs_10_3
		(0.87793-0.8829]	Rs_11_3
		(0.8829-0.88787]	Rs_12_3
		(0.88787-0.975]	Rs_13_3
		[0.983-1.02206]	Rs_14_3

Feature	Gradation	Feature	Gradation
		(1.02206-1.12]	Rs_15_3

It should be noted that great number of gradations for features is connected with closeness of crystal structures of colquirite, trirutile and Na_2SiF_6.

2.4.3. COMPUTER LEARNING AND PREDICTION OF CRYSTAL STRUCTURE

The computer learning is carried out for three learning sets in which the compounds from Table 2.4.1.1 were described in terms of the sets of the component properties 2.4.1, 2.4.2 and 2.4.3. The system of concept formation CONFOR [18-20] was used for computer learning and prediction.

The tables of predictions of the crystal structure type for the compounds of composition $ABCF_6$ (Tables 2.4.3.1 - 2.4.3.5) result from the comparison of the results of prediction with use of the descriptions in terms of the Features Sets 2.4.1, 2.4.2 and 2.4.3. The following designations are used:

L - colquirite ($LiCaAlF_6$);

N - Na_2SiF_6;

T - trirutile;

R - $RbNiCrF_6$;

C - $CsAgFeF_6$;

- - the crystal structure differing from those listed above;

* - the compound of composition $ABCF_6$ does not form.

The physical-chemical systems, which were investigated experimentally, were marked by round brackets. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. The designation "?" corresponds to the indeterminate result of predicring. According to our results the new compounds of the composition $LiCaCF_6$ (C = Sc, Mn, Cu, As, Y, or Tl), $LiVGaF_6$, $LiSrCF_6$ (C = Sc, Mn, Fe, Co, Cu, As, Y, Rh, or Tl), $LiCdCF_6$

(C = Al, Sc, Mn, Ni, Cu, Ga, As, Y, or Tl), $LiHgCF_6$ (C = V, Mn, Ni, Cu, or Ga), $LiPbCF_6$ (C = Mn, Ni, or Cu) have the colquirite crystal structure of at normal pressure and room temperature. We predicted new compounds of the composition $LiMnCF_6$ (C = Mn, As, Y, or Tl), $LiBInF_6$ (B = Ti, V, Cr, Fe, Cu, Pd, Ag, Hg, or Pb), $NaMgCF_6$ (C = Al, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Ga, As, Y, Rh, In, or Tl), $NaCaCF_6$ (C = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Ga, As, Y, Rh, In, or Tl), $NaTiCF_6$ (C = Al, Sc, V, Mn, Ga, As, Y, Rh, In, or Tl), $NaVCF_6$ (C = Al, Sc, Ti, Mn, Ga, As, Y, Rh, In, or Tl), $NaCrCF_6$ (C = Al, Sc, Ti, V, Mn, Ga, As, Y, Rh, or In), $NaMnCF_6$ (C = Sc, Ti, V, Ga, As, Y, Rh, In, or Tl), $NaFeCF_6$ (C = Al, Sc, Ti, V, Mn, Ga, As, Y, Rh, In, or Tl), $NaBCF_6$ (B = Co or Ni; C = Al, Sc, Ti, Ga, As, Y, Rh, In, or Tl), $NaCuCF_6$ (C = Al, Sc, Ti, V, Mn, Co, Ni, Ga, As, Y, Rh, or In), $NaZnCF_6$ (C = Al, Sc, Ti, Co, Ga, As, Y, Rh, In, or Tl), $NaSrCF_6$ (C = Sc, Ti, V, Mn, Co, Ni, Cu, Ga, As, Y, Rh, In, or Tl), $NaPdCF_6$ (C = Al, Sc, Ti, V, Mn, Ga, As, Y, Rh, In, or Tl), $NaAgCF_6$ (C = Al, Sc, Ti, V, Mn, Co, Ni, Cu, Ga, As, Y, Rh, In, or Tl), $NaCdCF_6$ (C = Sc, Ti, V, Mn, Co, Ni, Cu, Ga, As, Y, Rh, In, or Tl), $NaBaCF_6$ (C = Sc, Mn, Co, Ni, Cu, As, Y, Rh, In, or Tl), $NaBCF_6$ (B= Hg or Pb; C = Al, Sc, Ti, V, Mn, Co, Ni, Cu, Ga, As, Y, Rh, In, or Tl), $KTiVF_6$, $KCrVF_6$, $KMnCF_6$ (C = Al, Ti, V, Ga, As, Y, Rh, In, or Tl) with Na_2SiF_6 crystal structure at normal pressure and room temperature. These compounds hold the promise for searching for new EO, piezoelectric and non-linear materials. Compounds with Rb and Cs do not have crystal structures of colquirite and Na_2SiF_6 at normal pressure and room temperature.

Table 2.4.3.1

Table of Predictions of Crystal Structure Type
for Compounds of Composition LiBCF
6

B / C	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Pd	Ag	Cd	Ba	Hg	Pb
Al	(N)	(L)		N		(N)			?			(L)			L	(-)		
Sc	T	L	T	T	T	N	T	T	T	T	T	L	T	T	L	-		
Ti	(T)	(L)		T	T	(N)	(T)	(T)	(T)	T	(T)	(L)	T	T	(L)	(-)		
V	(T)	(L)				(N)		T	(T)	T	(T)	(L)			(L)	(-)	L	(L)
Cr	(T)	(L)	T	T		(N)	(T)	(T)	(T)	(T)	(T)	(L)	T	T	(L)	(-)		(L)
Mn	T	L	T	?	T		T	T	T	?	?	L	T	T	L	-	L	L
Fe	(T)	(L)	T	T	(T)	(N)	(T)	(T)	(T)	(T)	(T)	L	T	T	(L)	(-)		(L)
Co	(T)	(L)							T	(T)	(T)	L	T	T	(L)	(-)		
Ni	T	(L)		?							T	(L)	T	T	L	-	L	L
Cu	T	L		?							T	L	T	T	L	-	L	L
Ga	(T)	(L)		L		(N)	(N)	(T)	(T)	(T)		(L)			L	(-)	L	(L)
As	T	L	T	T	T	N	T	T	T	T	T	L	T	T	L	-		
Y	T	L	T	T	T	N	T	T	T	T	T	L	T	T	L	-		
Rh	(T)	(L)	T	T	T	(N)	T	(T)	(T)	(T)	(T)	L	T	T	(L)	-		
In	(N)	(N)	N	N	N	(N)	N	(N)	(N)	N	(N)	?	N	N	(N)	?	N	N
Tl	T	L	T	T		N	T	T	T		T	L	T	T	L	-		

Table 2.4.3.2

Table of Predictions of Crystal Structure Type
for Compounds of Composition NaBCF
6

B / C	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Pd	Ag	Cd	Ba	Hg	Pb
Al	N	(N)	N	N	N	(N)	N	N	N	N	N		N	N			N	N
Sc	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Ti	N	N		N	N	N	N	N	N	N	N	N	N	N	N		N	N
V	N	N	N	?	N	N	N	?	?	N	?	N	N	N	N		N	N
Cr	N	N	?	?		(N)	?	?	?	?	?	?	?	?	?	?	?	?
Mn	N	N	N	?	N		N	?	?	N	?	N	N	N	N	N	N	N
Fe	N	N	?	?	?	(N)	?	?	?	?	?	?	?	?	?	?	?	?
Co	N	N		?						N	N	N		N	N	N	N	N
Ni	N	N		?						N	?	N		N	N	N	N	N
Cu	N	N		?							?	N		N	N	N	N	N
Ga	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N		N	N
As	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Y	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Rh	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
In	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N	N
Tl	N	N	N	N		N	N	N	N		N	N	N	N	N	N	N	N

Table 2.4.3.3

Table of Predictions of Crystal Structure Type
for Compounds of Composition KBCF
6

B / C	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Pd	Ag	Cd	Ba	Hg	Pb
Al		*				N	-		(R)	*	*	*	*	*	*	*	*	*
Sc			*		-	?		*	*	*	*							
Ti		*				N	-			*	*	*	*	*	*	*	*	*
V	R	?	N		N	N	?	T	T	*	?	?	?	?	?	?	?	?
Cr	R	R	?	R		(-)	(-)	T	(R)	(-)	?	R	R	R	R	R	R	R
Mn	R	?	-	R	(-)		?	T	T	?	?	?	?	?	?	?	?	?
Fe	R	R	?	R	(-)	?		(-)	T	?	?	R	R	C	R	R	R	R
Co		*								*	*	*	*	*	*	*	*	*
Ni	R	*								*	?	?	?	?	?	?	?	?
Cu	R	*									?	?	?	?	?	?	?	?
Ga		*				N	-			*	*	*	*	*	*	*	*	*
As		*				N	-			*	*	*	*	*	*	*	*	*
Y		*				N	-			*	*	*	*	*	*	*	*	*
Rh		*				N	-			*	*	*	*	*	*	*	*	*
In	*			*		N		*	*	*	*							
Tl		*				N	-			*	*	*	*	*	*	*	*	*

Table 2.4.3.4

Table of Predictions of Crystal Structure Type
for Compounds of Composition RbBCF
6

B / C	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Pd	Ag	Cd	Ba	Hg	Pb
Al	(R)	C	C	C	C	?	C	C	(R)	(C)	C	C	C	(C)	C	C	C	C
Sc	R	C	C	C	C	?	C	R	R	R	R	C	C	C	C	C	C	C
Ti	R	C		C	C	?	C	R	R		R	C	C	C	C	C	C	C
V	R	C	?	?	?	?	(R)	?	?	(C)	?	C	C	C	C	C	C	C
Cr	(R)	?	?	?	?	(R)	(R)	(R)	(R)	(R)	(R)	C	?	C	C	C	C	C
Mn	R	C	?	?	(R)	?	C	?	?	?	(R)	C	C	C	C	C	C	C
Fe	R	?	?	(R)	(R)	(-)	?	R	(R)	(R)	R	C	?	(C)	C	C	C	C
Co	(R)	C				?			(R)	(R)	(R)	C		C	C	C	C	C
Ni	(R)	C	?	?	?	?				C	?	C		C	C	C	C	C
Cu	R	C	?	?	?	?		?	?		?	C		C	C	C	C	C
Ga	R	C	C	C	C	?	C	R	R		R	C	C	(C)	C	C	C	C
As	R	C	C	C	C	?	C	R	R		R	C	C	C	C	C	C	C
Y	R	C	C	C	C	?	C	R	R		R	C	C	C	C	C	C	C
Rh	R	C	C	C	C	?	C	R	R		R	C	C	C	C	C	C	C
In	R	C	C	C	C	?	C	R	R	R	R	C	C	C	C	C	C	C
Tl	R	C	C	C	C	?	C	R	R		R	C	C	C	C	C	C	C

Table 2.4.3.5

Table of Predictions of Crystal Structure Type
for Compounds of Composition CsBCF
6

B / C	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Pd	Ag	Cd	Ba	Hg	Pb
Al	(R)	R	R	R	R	R	R	?	(R)	C	(C)	R	R	(C)	R	R	R	R
Sc	R	R	R	(R)	R	R	R	R	R	R	R	R	(R)	(R)	R	R	R	R
Ti	(R)	R		R	R	R	R	(R)	(R)	(R)	(R)	R	R		R	R	R	R
V	(R)	R	R		(R)	(R)	(R)	(R)	(R)	(R)	(R)	R	R	R	R	R	R	R
Cr	(R)	R	R	(R)		(R)	(R)	(R)	(R)	(R)	(R)	R	R	R	R	R	R	R
Mn	R	R	?	(R)	(R)	?	R	?	(-)	R	(R)	R	R	R	R	R	R	R
Fe	(R)	R	R	(R)	(R)	(R)		(R)	(R)	(R)	(R)	R	(R)	(C)	R	R	R	R
Co	R	R							(R)	R	R	R			R	R	R	R
Ni	(R)	R	?		?	?				R	(R)	R		R	R	R	R	R
Cu	(R)	R	?		?	?				·	(R)	R			R	R	R	R
Ga	(R)	R	R	R	R	(R)	R	R	(R)	(R)	R	R	R	(C)	R	R	R	R
As	R	R	R	R	R	R	R	R	R	R	R	R	R		R	R	R	R
Y	R	R	R	R	R	R	R	R	R	R	R	R	R		R	R	R	R
Rh	R	R	R	R	R	R	R	R	R	R	R	R	(R)		R	R	R	R
In	R	R	R	R	R	R	R	R	(R)	(R)	(R)	R	(R)	(R)	R	R	R	R
Tl	R	R	R	R	R	R	R	R	R	(R)	R	R	R	(R)	R	R	R	R

2.5. PREDICTION OF NEW COMPOUNDS OF COMPOSITION $A^{I}B^{II}C^{III}F_7$

Complicated fluorides with composition $A^{I}BCF_7$ are of great interest because the experts suppose that they can have EO, nonlinear optical and piezoelectric properties [2,30]. For example, compounds $Na^{I}BCF_7$ have a transition ferroelectric->paraelectric above 700 K [30]. In addition, these crystals are piezoelectric and generate second harmonics at room temperature [30].

The most widespread for compounds $A^{I}B^{II}C^{III}F_7$ crystal structure types are: orthorhombic weberite ($Na^{I}MgAlF_7$, space group Imm2, Z=4), distorted trigonal weberite ($Na^{I}MnFeF_7$, space group P3 21, Z=6) and fluorite (space group Fm3m, Z=1).

In the structure of orthorhombic weberite the framework of octahedra contains B^{II} and C^{III} ions in different positions. The $(B^{II}F_{6/2})$ octahedra share trans corners to form chains along [100], which are linked together by isolated $(C^{III}F_{2}F_{4/2})$ octahedra possesing two terminal anions in a trans position. The 3D framework results from the intersection of layers which lie parallel to the (011) and $(\overline{011})$ planes of the lattice. The same layers occur in the trigonal weberites also [30,34].

The trigonal weberite structure is obviously favored by larger B^{II} ions. The main difference between the trigonal and orthorhombic types is that neihboring layers, which extend parallel to the trigonal plane, are rotated by 60° relative to each other. The $(C^{III}F_{2}F_{4/2})$ octahedron, which makes the interlayer connection, consequently has its terminal ligands in a cis position instead of a trans one [30].

The both types of weberites are of immediate interest for search for

new EO, nonlinear optical, lazer and piezoelectric materials [2,30]. But closeness of their crystal structures poses great difficulties for prediction of new compounds.

2.5.1. DATA FOR COMPUTER LEARNING

The data for computer learning was extracted from our the cardfile on quaternary inorganic compound properties. On the base of analysis of these data it may be concluded that only compounds A_2BCF_7 with A = Na and Ag can crystallize in weberite structure and Ag_2BCF_7 can crystallize in Na_2MnFeF_7. Therefore these structures at room state and normal pressure was predicted only for A = Na and Ag. The table 2.5.1.1 contains a learning set.

Table 2.5.1.1

Learning Set for Prediction of the Crystal Structure Type of Compounds with Composition A_2BCF_7

Composition	Crystal type
Na2MgAlF7	weberite
Na2MgScF7	weberite
Na2MgVF7	weberite
Na2MgCrF7	weberite
Na2MgFeF7	weberite
Na2MgGaF7	weberite
Na2MgInF7	weberite
Na2MgTlF7	weberite
Na2CoAlF7	weberite
Na2NiAlF7	weberite
Na2ZnAlF7	weberite
Na2CoScF7	weberite
Na2NiScF7	weberite
Na2CuScF7	weberite
Na2CoCrF7	weberite
Na2NiCrF7	weberite
Na2CuCrF7	weberite
Na2ZnCrF7	weberite
Na2MnTlF7	weberite
Na2CoFeF7	weberite
Na2NiFeF7	weberite
Na2CuFeF7	weberite

Composition	Crystal type
Na2ZnFeF7	weberite
Na2CoNiF7	weberite
Na2CoGaF7	weberite
Na2CoInF7	weberite
Na2NiGaF7	weberite
Na2NiInF7	weberite
Na2CuGaF7	weberite
Na2CuInF7	weberite
Na2ZnGaF7	weberite
Na2ZnInF7	weberite
Na2ZnTlF7	weberite
Ag2MgScF7	weberite
Ag2MgCrF7	weberite
Ag2MgFeF7	weberite
Ag2MgTlF7	weberite
Ag2MnAlF7	weberite
Ag2NiAlF7	weberite
Ag2CoCrF7	weberite
Ag2NiCrF7	weberite
Ag2CuCrF7	weberite
Ag2ZnCrF7	weberite
Ag2MnFeF7	weberite
Ag2FeMnF7	weberite
Ag2CuMnF7	weberite
Ag2ZnMnF7	weberite
Ag2CoFeF7	weberite
Ag2NiFeF7	weberite
Ag2CuFeF7	weberite
Ag2ZnFeF7	weberite
Ag2CoInF7	weberite
Ag2NiInF7	weberite
Ag2CuGaF7	weberite
Ag2CuInF7	weberite
Na2MnAlF7	Na2MnFeF7
Na2TiMnF7	Na2MnFeF7
Na2MnTiF7	Na2MnFeF7
Na2MnVF7	Na2MnFeF7
Na2VMnF7	Na2MnFeF7
Na2FeVF7	Na2MnFeF7
Na2VFeF7	Na2MnFeF7
Na2CrMnF7	Na2MnFeF7
Na2MnCrF7	Na2MnFeF7
Na2MnFeF7	Na2MnFeF7

Composition	Crystal type
Na2FeMnF7	Na2MnFeF7
Na2MnGaF7	Na2MnFeF7
Na2CaTmF7	Fluorite
Na2CaYbF7	Fluorite
Na2CaLuF7	Fluorite
Na2CdTmF7	Fluorite
Na2CdYbF7	Fluorite
Na2CdLuF7	Fluorite
Ag2CaErF7	Fluorite
Ag2CaTmF7	Fluorite
Ag2CaYbF7	Fluorite
Ag2CaLuF7	Fluorite
Ag2CdErF7	Fluorite
Ag2CdTmF7	Fluorite
Ag2CdYbF7	Fluorite
Ag2CdLuF7	Fluorite
NaF-BaF2-AlF3	without compound A2BCF7
NaF-PbF2-BiF3	without compound A2BCF7
KF-BeF2-LaF3	without compound A2BCF7
KF-CuF2-YbF3	without compound A2BCF7
KF-CuF2-LuF3	without compound A2BCF7
KF-CuF2-BiF3	without compound A2BCF7

2.5.2. SELECTION OF FEATURES

On the basis of physical-chemical grounds two sets of chemical elements features and set of simlpe fluorides feature were selected for the description of these systems.

2.5.2.1. FEATURE SET 2.5.1

The first feature set (feature set 2.5.1) includes information about the number of electrons in energy shells of isolated atoms and sum of Shannon effective ionic radii of element A with (C.N.=7) and with (C.N.=8), Shannon effective ionic radii of elements B (C.N.=6) and C (C.N.=6) in the compound of composition A_2BCF_7. The grouping of energy shell information corresponds to the number of electrons for each shell. The quasi-continuous properties - the ionic radii and sum of the ionic radii - were divided using the special program of discretization [18]. Table 2.5.2.1.1 contains the gradation for Feature Set

2.5.1.

Table 2.5.2.1.1

Gradations for Feature Set 2.5.1

Feature	Gradation	Feature	Gradation
	A-element		
3s-shell		4d-shell	
s1	s3_1_1	d0	d4_0_1
s2	s3_2_1	d10	d4_10_1
3p-shell		5s-shell	
p0	p3_0_1	s0	s5_0_1
p6	p3_6_1	s1	s5_1_1
3d-shell		Sum of Ionic	
d0	d3_0_1	radii, A	
d10	d3_10_1	[2.24-2.258]	R1_1
4s-shell		[2.354-2.384]	R2_1
s0	s4_0_1	[2.828-3.08]	R3_1
s2	s4_2_1		
4p-shell			
p0	p4_0_1		
p6	p4_6_1		
	B-element		
3s-shell		5s-shell	
s2	s3_2_2	s0	s5_0_2
3p-shell		s2	s5_2_2
p0	p3_0_2	5p-shell	
p6	p3_6_2	p0	p5_0_2
3d-shell		p6	p5_6_2
d0	d3_0_2	5d-shell	
d2	d3_2_2	d0	d5_0_2
d3	d3_3_2	d10	d5_10_2
d5	d3_5_2	6s-shell	
d6	d3_6_2	s0	s6_0_2
d7	d3_7_2	s2	s6_2_2
d8	d3_8_2	6p-shell	
d10	d3_10_2	p0	p6_0_2
4s-shell		p2	p6_2_2
s0	s4_0_2	Ionic	
s1	s4_1_2	radius, A	
s2	s4_2_2	[0.45-0.477]	R1_2
4p-shell		[0.675-0.729]	R2_2
p0	p4_0_2	(0.729-0.738]	R3_2
p6	p4_6_2	(0.738-0.765]	R4_2

Feature	Gradation	Feature	Gradation
4d-shell		(0.765-0.783]	R5_2
d0	d4_0_2	(0.783-0.819]	R6_2
d10	d4_10_2	(0.819-0.855]	R7_2
4f-shell		(0.855-0.882]	R8_2
f0	f4_0_2	[0.936-0.972]	R9_2
f14	f4_14_2	[0.99-1.026]	R10_2
		[1.17-1.215]	R11_2
		[1.323-1.35]	R12_2
	C-element		
3p-shell		5p-shell	
p1	p3_1_3	p0	p5_0_3
p6	p3_6_3	p1	p5_1_3
3d-shell		p6	p5_6_3
d0	d3_0_3	5d-shell	
d1	d3_1_3	d0	d5_0_3
d2	d3_2_3	d10	d5_10_3
d3	d3_3_3	6s-shell	
d5	d3_5_3	s0	s6_0_3
d6	d3_6_3	s2	s6_2_3
d7	d3_7_3	6p-shell	
d8	d3_8_3	p0	p6_0_3
d10	d3_10_3	p1	p6_1_3
4s-shell		Ionic	
s0	s4_0_3	radius, A	
s1	s4_1_3	[0.27-0.54991]	R1_3
s2	s4_2_3	(0.54991-0.61452]	R2_3
4p-shell		(0.61452-0.6344]	R3_3
p0	p4_0_3	(0.6344-0.64434]	R4_3
p1	p4_1_3	(0.64434-0.65925]	R5_3
p6	p4_6_3	(0.65925-0.6841]	R6_3
4d-shell		(0.6841-0.75865]	R7_3
d0	d4_0_3	(0.75865-0.81332]	R8_3
d1	d4_1_3	(0.81332-0.87793]	R9_3
d8	d4_8_3	(0.87793-0.8829]	R10_3
d10	d4_10_3	(0.8829-0.88787]	R11_3
4f-shell		(0.88787-0.9027799]	R12_3
f0	f4_0_3	(0.9027799-1.12]	R13_3
f14	f4_14_3		
5s-shell			
s0	s5_0_3		
s1	s5_1_3		
s2	s5_2_3		

2.5.2.2. FEATURE SET 2.5.2

The second feature set (feature set 2.5.2) includes the following information: the first three ionization potentials, the electronegativities by Pauling, the entropies of the individual substances at 298 K, the isobaric thermal capacities at 298 K, the temperatures and the heats of melting and boiling, Debye temperatures, the energies of the crystal lattice, sum of Shannon effective ionic radii of element A with (C.N.=7) and with (C.N.=8), Shannon effective ionic radii of elements B (C.N.=6) and C (C.N.=6), the ratio of the atomic number to the average atomic mass for atoms of elements A, B and C. The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.5.2.2.1 contains the gradations for Feature Set 2.5.2.

Table 2.5.2.2.1

Gradations for Feature Set 2.5.2

Feature	Gradation	Feature	Gradation
	A-element		
First ionization potential, eV		Boiling point, K	
[4.17717-4.437768]	I1_1_1	[963-1076.06]	Tb_1_1
[5.084888-5.214312]	I1_2_1	[1132.14-1188.22]	Tb_2_1
[7.479232-7.5763]	I1_3_1	[2393.94-2436]	Tb_3_1
Second ionization potential, eV		Heat of melting, kJ/mol	
[21.49-22.26391]	I2_1_1	[2.192-2.51424]	Hm_1_1
(22.26391-32.32474]	I2_2_1	(2.51424-2.7831]	Hm_2_1
[46.77106-47.287]	I2_3_1	[11.02814-11.297]	Hm_3_1
Third ionization potential, eV		Heat of boiling, kJ/mol	
[34.8-35.9046]	I3_1_1	[80.751-93.42075]	Hb_1_1
(35.9046-46.5824]	I3_2_1	[103.1962-111.3425]	Hb_2_1
[70.88361-71.62]	I3_3_1	[248.1995-251.458]	Hb_3_1
Electronegativity		Energy of the crystal lattice,	
[0.8-0.833]	X_1_1	-6	
[0.877-0.932]	X_2_1	E*10 J/kg*mol	
[1.878-1.9]	X_3_1	[86-96.194]	E_1_1
Entropies of individual		[104.186-114.176]	E_2_1
substances at 298 K		[286.00-4290]	E_3_1
kJ/kg*mol*K		Debye temperature, K	
[42.551-43.21502]	S_1_1	[55-94.05]	Td_1_1

Feature	Gradation	Feature	Gradation
[50.74058-51.84728]	S_2_1	[156.15-162.9]	Td_2_1
[64.24232-76.735]	S_3_1	[222.3-225]	Td_3_1
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		Ratio of the atomic number to the average atomic mass	
[25.355-25.48052]	Cp_1_1		
[28.0746-28.2838]	Cp_2_1	[0.43-0.4415]	NM_1_1
[29.45532-31.045]	Cp_3_1	[0.4785-0.481]	NM_2_1
Melting point, K		[0.489-0.49]	NM_3_1
[312.47-363.5802]	Tm_1_1	Sum of Ionic radius, A	
(363.5802-390.5004]	Tm_2_1		
[1216.053-1234]	Tm_3_1	[2.24-2.258]	Rs_1_1
		[2.354-2.384]	Rs_2_1
		[2.828-3.08]	Rs_3_1
	B-element		
First ionization potential, eV		Boiling point, K	
		[630-1118.86]	Tb_1_2
[5.21166-5.337139]	I1_1_2	(1118.86-1250.878]	Tb_2_2
(5.337139-6.215494]	I1_2_2	[1303.685-1435.703]	Tb_3_2
(6.215494-6.926542]	I1_3_2	(1435.703-1831.755]	Tb_4_2
[7.344807-7.428459]	I1_4_2	[1990.176-2201.404]	Tb_5_2
(7.428459-7.553938]	I1_5_2	[2307.018-2412.632]	Tb_6_2
(7.553938-7.721244]	I1_6_2	(2412.632-2808.685]	Tb_7_2
(7.721244-7.846724]	I1_7_2	(2808.685-2887.895]	Tb_8_2
(7.846724-7.88855]	I1_8_2	(2887.895-3019.913]	Tb_9_2
(7.88855-8.014029]	I1_9_2	[3072.719-3151.93]	Tb_10_2
(8.014029-9.101516]	I1_10_2	(3151.93-3283.948]	Tb_11_2
[9.268821-9.352474]	I1_11_2	[3547.982-4100]	Tb_12_2
(9.352474-10.4376]	I1_12_2	Heat of melting, kJ/mol	
Second ionization potential, eV		[2.295-5.324186]	Hm_1_2
[10.004-10.31267]	I2_1_2	[5.688883-6.600626]	Hm_2_2
(10.31267-12.16469]	I2_2_2	(6.600626-7.147672]	Hm_3_2
(12.16469-13.81093]	I2_3_2	(7.147672-7.694717]	Hm_4_2
[14.42827-14.94272]	I2_4_2	[8.059415-8.971158]	Hm_5_2
(14.94272-15.25139]	I2_5_2	(8.971158-12.43578]	Hm_6_2
[15.45717-15.86873]	I2_6_2	(12.43578-12.80048]	Hm_7_2
(15.86873-16.48607]	I2_7_2	(12.80048-13.34752]	Hm_8_2
(16.48607-16.79474]	I2_8_2	(13.34752-14.25927]	Hm_9_2
(16.79474-17.00052]	I2_9_2	[14.62396-15.53571]	Hm_10_2
(17.00052-17.30919]	I2_10_2	[15.9004-16.81215]	Hm_11_2
[17.72075-18.13231]	I2_11_2	[17.17684-17.90624]	Hm_12_2

Feature	Gradation	Feature	Gradation
(18.13231-18.44098]	I2_12_2	(17.90624-21.37086]	Hm_13_2
(18.44098-21.49]	I2_13_2	[22.46495-31.81968]	Hm_14_2
Third ionization potential, eV		Heat of boiling, kJ/mol	
[24.9-30.0182]	I3_1_2	[59.229-109.9344]	Hb_1_2
(30.0182-31.2823]	I3_2_2	(109.9344-123.7416]	Hb_2_2
(31.2823-32.5464]	I3_3_2	[137.5488-151.356]	Hb_3_2
(32.5464-38.8669]	I3_4_2	(151.356-175.5186]	Hb_4_2
(38.8669-42.6592]	I3_5_2	(175.5186-185.874]	Hb_5_2
(42.6592-54.0361]	I3_6_2	[220.392-234.1992]	Hb_6_2
[76.7899-83.1104]	I3_7_2	(234.1992-310.1388]	Hb_7_2
[151.3718-153.9]	I3_8_2	(310.1388-323.946]	Hb_8_2
Electronegativity		[330.8496-348.1086]	Hb_9_2
[0.9-0.9299999]	X_1_2	(348.1086-358.464]	Hb_10_2
[0.97-1.02]	X_2_2	[365.3676-382.6266]	Hb_11_2
(1.02-1.23]	X_3_2	[403.3374-420.5964]	Hb_12_2
[1.47-1.52]	X_4_2	[434.4036-510.448]	Hb_13_2
[1.58-1.63]	X_5_2	Energy of the crystal lattice, -6 E*10 J/kg*mol	
[1.69-1.73]	X_6_2		
[1.77-1.82]	X_7_2		
[1.88-2.2]	X_8_2		
Entropies of individual substances at 298 K kJ/kg*mol*K		[116-127.61]	E_1_2
		(127.61-158.57]	E_2_2
		(158.57-185.66]	E_3_2
		(185.66-205.01]	E_4_2
[9.498-11.24598]	S_1_2	[274.67-294.02]	E_5_2
[22.89918-25.22982]	S_2_2	[317.24-332.72]	E_6_2
[26.39514-28.72578]	S_3_2	(332.72-340.46]	E_7_2
(28.72578-29.30844]	S_4_2	(340.46-352.07]	E_8_2
(29.30844-30.47376]	S_5_2	(352.07-413.99]	E_9_2
(30.47376-31.63908]	S_6_2	[421.73-441.08]	E_10_2
(31.63908-32.22174]	S_7_2	[464.3-479.78]	E_11_2
(32.22174-32.8044]	S_8_2	[495.26-510]	E_12_2
(32.8044-34.55238]	S_9_2	Debye temperature, K	
(34.55238-43.29228]	S_10_2		
[50.2842-53.1975]	S_11_2	[75-126.95]	Td_1_2
(53.1975-63.68538]	S_12_2	(126.95-244.1]	Td_2_2
[66.01602-79.898]	S_13_2	(244.1-329.3]	Td_3_2
Isobaric thermal capacity at 298 K, kJ/kg*mol*K		(329.3-371.9]	Td_4_2
		(371.9-403.85]	Td_5_2
		(403.85-425.15]	Td_6_2
[16.443-16.79196]	Cp_1_2	(425.15-435.8]	Td_7_2
[23.07324-23.65484]	Cp_2_2	(435.8-446.45]	Td_8_2

Feature	Gradation	Feature	Gradation
[24.12012-24.70172]	Cp_3_2	(446.45-457.1]	Td_9_2
(24.70172-24.81804]	Cp_4_2	(457.1-489.05]	Td_10_2
(24.81804-24.93436]	Cp_5_2	[574.25-616.85]	Td_11_2
(24.93436-25.05068]	Cp_6_2	[1128.05-1160]	Td_12_2
(25.05068-25.39964]	Cp_7_2	Ratio of the	
(25.39964-25.7486]	Cp_8_2	atomic number	
(25.7486-25.98124]	Cp_9_2	to the average	
(25.98124-26.21388]	Cp_10_2	atomic mass	
(26.21388-26.3302]	Cp_11_2	[0.4-0.403]	NM_1_2
(26.3302-26.67916]	Cp_12_2	[0.407-0.412]	NM_2_2
(26.67916-28.075]	Cp_13_2	[0.428-0.432]	NM_3_2
Melting point, K		[0.438-0.442]	NM_4_2
[234.29-641.88]	Tm_1_2	[0.448-0.452]	NM_5_2
[673.8-737.64]	Tm_2_2	[0.458-0.462]	NM_6_2
[897.24-961.08]	Tm_3_2	[0.468-0.472]	NM_7_2
(961.08-1040.88]	Tm_4_2	[0.478-0.482]	NM_8_2
(1040.88-1152.6]	Tm_5_2	[0.488-0.492]	NM_9_2
(1152.6-1392]	Tm_6_2	[0.498-0.5]	NM_10_2
[1519.68-1599.48]	Tm_7_2	Ionic radius, A	
[1695.24-1806.96]	Tm_8_2	[0.45-0.477]	Rs_1_2
(1806.96-1854.84]	Tm_9_2	[0.675-0.729]	Rs_2_2
[1918.68-1982.52]	Tm_10_2	(0.729-0.738]	Rs_3_2
(1982.52-2190]	Tm_11_2	(0.738-0.765]	Rs_4_2
		(0.765-0.783]	Rs_5_2
		(0.783-0.819]	Rs_6_2
		(0.819-0.855]	Rs_7_2
		(0.855-0.882]	Rs_8_2
		[0.936-0.972]	Rs_9_2
		[0.99-1.026]	Rs_10_2
		[1.17-1.21]	Rs_11_2
		[1.323-1.3]	Rs_12_2
	C-element		
First ionization potential, eV		Boiling point, K	
		[885-1655.61]	Tb_1_3
[5.2-5.500292]	I1_1_3	[1697.35-1801.7]	Tb_2_3
(5.500292-5.648876]	I1_2_3	(1801.7-1885.18]	Tb_3_3
(5.648876-5.846988]	I1_3_3	(1885.18-2052.14]	Tb_4_3
(5.846988-6.16892]	I1_4_3	[2260.84-2344.32]	Tb_5_3
(6.16892-6.243212]	I1_5_3	(2344.32-2406.93]	Tb_6_3
(6.243212-6.317504]	I1_6_3	(2406.93-2532.15]	Tb_7_3
[6.515616-6.614672]	I1_7_3	(2532.15-2740.85]	Tb_8_3
[6.713728-6.763256]	I1_8_3	(2740.85-2845.2]	Tb_9_3

Feature	Gradation	Feature	Gradation
(6.763256-6.812784]	I1_9_3	(2845.2-2949.55]	Tb_10_3
(6.812784-6.887076]	I1_10_3	(2949.55-3012.16]	Tb_11_3
(6.887076-7.357592]	I1_11_3	(3012.16-3158.25]	Tb_12_3
(7.357592-7.506176]	I1_12_3	(3158.25-3220.86]	Tb_13_3
(7.506176-7.704288]	I1_13_3	(3220.86-3325.21]	Tb_14_3
(7.704288-9.789]	I1_14_3	(3325.21-3638.26]	Tb_15_3
Second ionization		(3638.26-3659.13]	Tb_16_3
potential, eV		(3659.13-5770]	Tb_17_3
[10.6-11.38245]	I2_1_3	Heat of melting,	
(11.38245-12.13565]	I2_2_3	kJ/mol	
(12.13565-12.4181]	I2_3_3	[2.8-4.84384]	Hm_1_3
[12.6064-13.07715]	I2_4_3	[5.2388-6.02872]	Hm_2_3
[13.45375-13.83035]	I2_5_3	[8.79344-9.78084]	Hm_3_3
(13.83035-14.1128]	I2_6_3	(9.78084-10.96572]	Hm_4_3
(14.1128-14.866]	I2_7_3	(10.96572-11.75564]	Hm_5_3
[15.4309-15.90165]	I2_8_3	(11.75564-12.54556]	Hm_6_3
[16.08995-16.65485]	I2_9_3	(12.54556-14.32288]	Hm_7_3
(16.65485-16.9373]	I2_10_3	(14.32288-15.50776]	Hm_8_3
(16.9373-18.4437]	I2_11_3	[15.90272-16.69264]	Hm_9_3
(18.4437-19.10275]	I2_12_3	(16.69264-17.48256]	Hm_10_3
(19.10275-25.155]	I2_13_3	(17.48256-18.075]	Hm_11_3
Third ionization		(18.075-18.86492]	Hm_12_3
potential, eV		(18.86492-19.65484]	Hm_13_3
[19.18-19.6636]	I3_1_3	(19.65484-21.43216]	Hm_14_3
(19.6636-21.4368]	I3_2_3	[21.548-52]	Hm_15_3
(21.4368-23.0488]	I3_3_3	Heat of boiling,	
[23.3712-24.1772]	I3_4_3	kJ/mol	
[24.4996-24.9832]	I3_5_3	[31.798-173.0177]	Hb_1_3
(24.9832-25.4668]	I3_6_3	(173.0177-175.7906]	Hb_2_3
(25.4668-25.9504]	I3_7_3	(175.7906-184.1092]	Hb_3_3
(25.9504-27.8848]	I3_8_3	(184.1092-234.0209]	Hb_4_3
(27.8848-28.3684]	I3_9_3	[239.5666-250.6581]	Hb_5_3
(28.3684-28.852]	I3_10_3	(250.6581-261.7496]	Hb_6_3
(28.852-29.658]	I3_11_3	[289.4783-300.5698]	Hb_7_3
(29.658-30.3028]	I3_12_3	(300.5698-325.5256]	Hb_8_3
(30.3028-31.4312]	I3_13_3	(325.5256-339.39]	Hb_9_3
(31.4312-34.0104]	I3_14_3	(339.39-356.0272]	Hb_10_3
(34.0104-37.931]	I3_15_3	(356.0272-375.4373]	Hb_11_3
Electronegativity		(375.4373-417.0303]	Hb_12_3
[1.1-1.124]	X_1_3	(417.0303-425.3489]	Hb_13_3
(1.124-1.316]	X_2_3	[436.4404-744.752]	Hb_14_3
[1.476-1.516]	X_3_3	Energy of the	
[1.58-1.62]	X_4_3	crystal lattice,	

Feature	Gradation	Feature	Gradation
[1.684-1.724]	X_5_3	-6	
[1.788-1.82]	X_6_3	E*10 J/kg*mol	
[1.884-2.4]	X_7_3	[182.8-192.406]	E_1_3
Entropies of		[198.81-214.82]	E_2_3
individual		[240.436-253.244]	E_3_3
substances at 298 K		(253.244-285.264]	E_4_3
kJ/kg*mol*K		(285.264-294.87]	E_5_3
[5.853-25.12636]	S_1_3	[307.678-323.688]	E_6_3
[26.11726-28.59452]	S_2_3	[330.092-346.102]	E_7_3
(28.59452-29.58543]	S_3_3	(346.102-368.516]	E_8_3
(29.58543-30.57634]	S_4_3	(368.516-378.122]	E_9_3
(30.57634-31.56724]	S_5_3	[384.526-397.334]	E_10_3
(31.56724-33.0536]	S_6_3	(397.334-413.344]	E_11_3
(33.0536-38.99903]	S_7_3	[419.748-432.556]	E_12_3
[39.98993-42.4672]	S_8_3	[464.576-477.384]	E_13_3
[42.0548-50.39444]	S_9_3	[496.596-775]	E_14_3
(50.39444-57.33078]	S_10_3	Debye	
(57.33078-58.81713]	S_11_3	temperature, K	
[61.78985-63.77166]	S_12_3	[89-93.96]	Td_1_3
(63.77166-65.25802]	S_13_3	(93.96-108.84]	Td_2_3
(65.25802-74.81812]	S_14_3	(108.84-113.8]	Td_3_3
Isobaric thermal		(113.8-143.56]	Td_4_3
capacity at 298 K,		(143.56-163.4]	Td_5_3
kJ/kg*mol*K		(163.4-178.28]	Td_6_3
[11.088-21.00648]	Cp_1_3	(178.28-346.92]	Td_7_3
[23.21127-23.50524]	Cp_2_3	[366.76-391.56]	Td_8_3
(23.50524-24.53414]	Cp_3_3	[411.4-426.28]	Td_9_3
(24.53414-24.9751]	Cp_4_3	(426.28-441.16]	Td_10_3
(24.9751-25.04859]	Cp_5_3	(441.16-461]	Td_11_3
(25.04859-25.12209]	Cp_6_3	(461-465.96]	Td_12_3
(25.12209-25.34257]	Cp_7_3	(465.96-480.84]	Td_13_3
(25.34257-26.22448]	Cp_8_3	[570.12-1219]	Td_14_3
(26.22448-26.29797]	Cp_9_3	Ratio of the	
(26.29797-26.88592]	Cp_10_3	atomic number	
(26.88592-27.17989]	Cp_11_3	to the average	
(27.17989-28.06181]	Cp_12_3	atomic mass	
(28.06181-36.5089]	Cp_13_3	[0.39-0.4024]	NM_1_3
Melting point, K		[0.4088-0.412]	NM_2_3
[303-359.61]	Tm_1_3	(0.412-0.432]	NM_3_3
[397.35-472.83]	Tm_2_3	[0.4384-0.4416]	NM_4_3
[510.57-567.18]	Tm_3_3	[0.448-0.452]	NM_5_3
(567.18-623.79]	Tm_4_3	[0.4584-0.4624]	NM_6_3
[887.97-982.32]	Tm_5_3	[0.4688-0.472]	NM_7_3

Feature	Gradation	Feature	Gradation
[1057.8-1152.15]	Tm_6_3	[0.4784-0.48]	NM_8_3
(1152.15-1246.5]	Tm_7_3	Ionic radius, A	
(1246.5-1605.03]	Tm_8_3	[0.27-0.54991]	Rs_1_3
(1605.03-1755.99]	Tm_9_3	(0.54991-0.61452]	Rs_2_3
(1755.99-1793.73]	Tm_10_3	(0.61452-0.6344]	Rs_3_3
(1793.73-1812.6]	Tm_11_3	(0.6344-0.64434]	Rs_4_3
(1812.6-1869.21]	Tm_12_3	(0.64434-0.65925]	Rs_5_3
[1906.95-1982.43]	Tm_13_3	(0.65925-0.6841]	Rs_6_3
[2133.39-2171.13]	Tm_14_3	(0.6841-0.75865]	Rs_7_3
(2171.13-3287]	Tm_15_3	(0.75865-0.81332]	Rs_8_3
		(0.81332-0.87793]	Rs_9_3
		(0.87793-0.8829]	Rs_10_3
		(0.8829-0.88787]	Rs_11_3
		(0.88787-0.9027799]	Rs_12_3
		(0.9027799-1.12]	Rs_13_3

2.5.2.3. FEATURE SET 2.5.3

The third set of properties of simple fluorides (feature set 2.5.3) includes the following information of simple fluorides AF_2, BF_3 and CF_4 : the melting point, standard enthalpy of formation, standard isobaric thermal capacities, standard entropies, sum of Shannon effective ionic radii of element A with (C.N.=7) and with (C.N.=8), Shannon effective ionic radii of correspoding cations B^{2+} (C.N.=6) and C^{3+} (C.N.=6). The all quasi-continuous properties were divided using the special program of discretization [18]. Table 2.5.2.3.1 contains the gradations for Feature Set 2.5.3.

Table 2.5.2.3.1

Gradations for Feature Set 2.5.3
(Properties of Simple Fluorides)

Feature	Gradation	Feature	Gradation
	AF		
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[49.9-52.5103]	H_1_1	[11.19-11.518]	Cp_1_1
[132.83-136.0399]	H_2_1	[11.71-11.734]	Cp_2_1
(136.0399-136.91]	H_3_1	[12.082-12.1]	Cp_3_1
Standard entropy for corresponding simple fluorides, cal/mol*K		Melting point of simple fluorides, K	
[12.23-12.4631]	So_1_1	[708-724.8]	Tm_1_1
[15.7265-16.115]	So_2_1	(724.8-1144.8]	Tm_2_1
(16.115-20]	So_3_1	[1256.8-1268]	Tm_3_1
		Sum of ionic radii, A	
		[2.24-2.258]	Rs_1_1
		[2.354-2.384]	Rs_2_1
		[2.828-3.08]	Rs_3_1
	BF 2		
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[82-133.399]	H_1_2	[12.39-12.5493]	Cp_1_2
[140-157.894]	H_2_2	[14.1423-14.3547]	Cp_2_2
(157.894-161.16]	H_3_2	[14.5671-14.8326]	Cp_3_2
(161.16-166.059]	H_4_2	[15.1512-15.4167]	Cp_4_2
(166.059-170.958]	H_5_2	[15.6291-15.8415]	Cp_5_2
[180.756-184.022]	H_6_2	[15.9477-16.1601]	Cp_6_2
(184.022-188.921]	H_7_2	(16.1601-16.2663]	Cp_7_2
[195.453-201.985]	H_8_2	(16.2663-16.4256]	Cp_8_2
(201.985-206.884]	H_9_2	(16.4256-16.5849]	Cp_9_2
[242.81-249.342]	H_10_2	[16.6911-16.9566]	Cp_10_2
[265.672-272.204]	H_11_2	(16.9566-17.1159]	Cp_11_2
		[17.5407-17.7]	Cp_12_2

Feature	Gradation	Feature	Gradation
[278.736-286.901]	H_12_2	Melting point of	
(286.901-291.8]	H_13_2	simple fluorides, K	
Standard entropy		[385-1062.44]	Tm_1_2
for corresponding		(1062.44-1114.28]	Tm_2_2
simple fluorides,		(1114.28-1146.68]	Tm_3_2
cal/mol*K		(1146.68-1166.12]	Tm_4_2
[12.75-13.1775]	So_1_2	(1166.12-1185.56]	Tm_5_2
[13.4625-14.0325]	So_2_2	[1225-1360.52]	Tm_6_2
[16.0275-16.74]	So_3_2	(1360.52-1392.92]	Tm_7_2
[17.31-17.88]	So_4_2	(1392.92-1444.76]	Tm_8_2
(17.88-18.3075]	So_5_2	[1522.52-1548.44]	Tm_9_2
[18.8775-19.4475]	So_6_2	(1548.44-1567.88]	Tm_10_2
(19.4475-19.875]	So_7_2	[1580.84-1593.8]	Tm_11_2
(19.875-20.3025]	So_8_2	(1593.8-1613.24]	Tm_12_2
(20.3025-20.73]	So_9_2	[1673-1691]	Tm_13_2
(20.73-21.1575]	So_10_2	Ionic radii, A	
[22.0125-22.5825]	So_11_2	[0.45-0.477]	Rs_1_2
[22.8675-23.4375]	So_12_2	[0.675-0.729]	Rs_2_2
[24-27]	So_13_2	(0.729-0.738]	Rs_3_2
		(0.738-0.765]	Rs_4_2
		(0.765-0.783]	Rs_5_2
		(0.783-0.819]	Rs_6_2
		(0.819-0.855]	Rs_7_2
		(0.855-0.882]	Rs_8_2
		[0.936-0.972]	Rs_9_2
		[0.9901.026]	Rs_10_2
		[1.1701.215]	Rs_11_2
		[1.32301.35]	Rs_12_2
	CF 3		
Standard enthalpy		Standard isobaric	
of formation for		thermal capacity	
corresponding		for simple fluorides,	
simple fluorides,		cal/mol*K	
kcal/mol		[8.22-8.622001]	Cp_1_3
[122-182.167]	H_1_3	[17.734-18.27]	Cp_2_3
(182.167-222.78]	H_2_3	[18.538-19.208]	Cp_3_3
(222.78-244.281]	H_3_3	[21.352-30.25]	Cp_4_3
(244.281-253.837]	H_4_3	Melting point of	
(253.837-261.004]	H_5_3	simple fluorides, K	
[265.782-275.338]	H_6_3	[267-853.06]	Tm_1_3
(275.338-282.505]	H_7_3	[973.3-1023.4]	Tm_2_3

Feature	Gradation	Feature	Gradation
[339.841-349.397]	H_8_3	[1203.76-1253.86]	Tm_3_3
[354.175-366.12]	H_9_3	[1273.9-1324]	Tm_4_3
(366.12-394.788]	H_10_3	(1324-1374.1]	Tm_5_3
(394.788-411.511]	H_11_3	[1394.14-1434.22]	Tm_6_3
(411.511-414.1]	H_12_3	(1434.22-1444.24]	Tm_7_3
Standard entropy		(1444.24-1454.26]	Tm_8_3
for corresponding		(1454.26-1484.32]	Tm_9_3
simple fluorides,		(1484.32-1524.4]	Tm_10_3
cal/mol*K		(1524.4-1574.5]	Tm_11_3
[15.89-17.1629]	So_1_3	(1574.5-1704.76]	Tm_12_3
(17.1629-18.8601]	So_2_3	(1704.76-1794.94]	Tm_13_3
[20.5573-22.2545]	So_3_3	(1794.94-1825]	Tm_14_3
(22.2545-23.1031]	So_4_3	Ionic radii, A	
(23.1031-23.9517]	So_5_3	[0.27-0.54991]	Rs_1_3
(23.9517-24.8003]	So_6_3	(0.54991-0.6344]	Rs_2_3
(24.8003-26.0732]	So_7_3	(0.6344-0.64434]	Rs_3_3
(26.0732-27.7704]	So_8_3	(0.64434-0.65925]	Rs_4_3
(27.7704-28.619]	So_9_3	(0.65925-0.6841]	Rs_5_3
(28.619-29.8919]	So_10_3	(0.6841-0.75865]	Rs_6_3
(29.8919-34.9835]	So_11_3	(0.75865-0.81332]	Rs_7_3
(34.9835-60.7]	So_12_3	[0.85308-0.87793]	Rs_8_3
		(0.87793-0.8829]	Rs_9_3
		(0.8829-0.88787]	Rs_10_3
		(0.88787-0.9027799]	Rs_11_3
		(0.9027799-1.61]	Rs_12_3

It should be noted that great number of gradations for features is connected with closeness of crystal structures of orthorhombic and trigonal weberites.

2.5.3. COMPUTER LEARNING AND PREDICTION OF CRYSTAL STRUCTURE

The computer learning is carried out for three learning sets in which the compounds from Table 2.5.1.1 were described in terms of the sets of the component properties 2.5.1, 2.5.2 and 2.5.3. The system of concept formation CONFOR [18-20] was used for computer learning and prediction.

The tables of predictions of the crystal structure type for the compounds of composition A_2BCF_7 (Tables 2.5.3.1 and 2.5.3.2) result from the comparison of the results of prediction with use of the descrip-

tions in terms of the Features Sets 2.5.1, 2.5.2 and 2.5.3. The following designations are used:

W - orthorhombic weberite;
N - trigonal weberite;
F - fluorite;
* - the compound of composition A_2BCF_7 does not form.

The physical-chemical systems, which were investigated experimentally, were marked by round brackets. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. The designation "?" corresponds to the indeterminate result of predicring. According to our results the new compounds of the composition Na_2MgCF_7 (C = Ti, Mn, Co, Ni, Y, or Rh), Na_2CaCF_7 (C = Sc, Ga, In, or Tl), Na_2BCF_7 (B = Ti or V; C = Sc, Ga, or In), Na_2CrCF_7 (C = Ga or In), Na_2MnInF_7, Na_2BCF_7 (B = Co or Ni; C = Ti, V, Mn, Y, Rh, or Tl), Na_2CuCF_7 (C = Ti, V, Mn, Co, or Ni), Na_2ZnCF_7 (C = Sc, Ti, V, Mn, Co, Ni, Y, or Rh), Na_2BCF_7 (B = Sr or Cd; C = Sc, Cr, Ga, In, or Tl), Na_2BCF_7 (B = Ba, Hg, or Pb; C = Sc, Cr, Ga, or In), Ag_2MgCF_7 (C = Al, Ti, V, Mn, Co, Ni, Ga, Y, Rh, or In), Ag_2CaCF_7 (C = Al, Sc, Cr, Mn, Fe, Co, Ni, or Ga), Ag_2BCF_7 (B = Ti or V; C = Al, Sc, Cr, Mn, Fe, Ga, or Tl), Ag_2CrCF_7 (C = Al, Sc, Mn, Fe, Ga, or Tl), Ag_2MnCF_7 (C = Sc, Cr, Ga, or Tl), Ag_2FeCF_7 (C = Al, Sc, Ti, V, Cr, Ga, Y, Rh, In, or Tl), Ag_2CoCF_7 (C = Al, Sc, Ti, V, Mn, Ga, Y, Rh, or Tl), Ag_2NiCF_7 (C = Sc, Ti, V, Mn, Ga, Y, Rh, or Tl), Ag_2CuCF_7 (C = Al, Sc, Ti, V, Co, Ni, Y, Rh, or Tl), Ag_2ZnCF_7 (C= Al, Sc, Ti, V, Co, Ni, Ga, Y, Rh, In, or Tl), Ag_2BCF_7 (B = Sr, Cd, Ba, Hg, or Pb; C = Al, Sc, Cr, Mn, Fe, Ni, Ga, or In) and Ag_2PdCF_7 (C = Al, Sc, Cr, Mn, Fe, Ga, or In)* have the orthorhombic weberite crystal structure of at normal pressure and room temperature. We pre-

dicted the new compounds of the composition Na_2CaCF_7 (C = Ti, V, Mn, Fe, Co, Ni, or Rh), Na_2TiCF_7 (C = V, Fe, or Rh), Na_2VCF_7 (C = Ti or Rh), Na_2CrCF_7 (C = Ti, V, Fe, or Rh), Na_2MnRhF_7, Na_2FeCF_7 (C = Al, Ti, V, Cr, Mn, Y, or Rh) and Na_2BCF_7 (B = Sr, Cd, Ba, Hg, or Pb; C = Ti, V, Mn, Fe, Co, or Rh) with trigonal weberite crystal structure of at normal pressure and room temperature also. The compounds with silver do not crystillize at normal state in trigonal weberite crystal structure. Compounds with weberite structure hold the promise for searching for new EO, piezoelectric, lazer and nonlinear materials.

Table 2.5.3.1

Table of Predictions of Crystal Structure Type
for Compounds of Composition Na BCF
2 7

B / C	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Cd	Ba	Hg	Pb
Al	(W)					(N)	N	(W)	(W)	W	(W)			(*)		
Sc	(W)	W	W	W			?	(W)	(W)	(W)	W	W	W	W	W	W
Ti	(W)	N		N	N	(N)	N	W	W	W	N	N	N	N	N	N
V	(W)	N	N		N	(N)	N	W	W	W	N	N	N	N	N	N
Cr	(W)					(N)	N	(W)	(W)	(W)	(W)	W	W	W	W	W
Mn	W	N	(N)	(N)	(N)		N	W	W	W	W	N	N	N	N	N
Fe	(W)	N	N	(N)	N	(N)		(W)	(W)	(W)	(W)	N	N	N	N	N
Co	W	N							(W)	W	W	N	N	N	N	N
Ni	W	N						(W)		W	W	?	?	?	?	?
Ga	(W)	W	W	W	W	(N)	?	(W)	(W)	(W)	(W)	W	W	W	W	W
Y	W						N	W	W		W					
Rh	W	N	N	N	N	N	N	W	W		W	N	N	N	N	N
In	(W)	W	W	W	W	W	?	(W)	(W)	(W)	(W)	W	W	W	W	W
Tl	(W)	W				(W)	?	W	W		(W)	W	W			

Table 2.5.3.2

Table of Predictions of Crystal Structure Type
for Compounds of Composition Ag BCF
2 7

B / C	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Pd	Cd	Ba	Hg	Pb
Al	W	W	W	W	W	(W)	W	W	(W)	W	W	W	W	W	W	W	W
Sc	(W)	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W	W
Ti	W						W	W	W	W	W	F	F	F	F	F	F
V	W						W	W	W	W	W	F	F	F	F	F	F
Cr	(W)	W	W	W		W	W	(W)	(W)	(W)	(W)	W	W	W	W	W	W
Mn	W	W	W	W	W		(W)	W	W	(W)	(W)	W	W	W	W	W	W
Fe	(W)	W	W	W	W	(W)		(W)	(W)	(W)	(W)	W	W	W	W	W	W
Co	W	W								W	W	?	?	?	?	?	?
Ni	W	W								W	W	W		W	W	W	W
Ga	W	W	W	W	W	W	W	W	W	(W)	W	W	W	W	W	W	W
Y	W						W	W	W	W	W	F	F	F	F	?	?
Rh	W						W	W	W	W	W						
In	W						W	(W)	(W)	(W)	W	W	W	W	W	W	W
Tl	(W)		W	W	W	W	W	W	W	W						-	

3. TEST OF DISCRETIZATION PROGRAM

In order to test an efficiency of developed program of discretization we chose a number of task using table of random numbers (an uniform distribution). This task is a prediction of crystal structure types
I II III
for compounds A B C F (using the simple fluorides properties).
6
The learning set included 113 objects (Table 3.1) and set for exami-

nation included 76 objects (Table 3.2). The numbers of objects for examination were chosen using the table of random numbers (an uniform distribution).

Table 3.1

Learning Set

Composition	Crystal type	Space group
LiMgAlF6	Na2SiF6	
LiMnAlF6	Na2SiF6	
LiCaInF6	Na2SiF6	
LiMnTiF6	Na2SiF6	
LiMnVF6	Na2SiF6	
LiMnCrF6	Na2SiF6	
LiMnRhF6	Na2SiF6	
LiFeGaF6	Na2SiF6	
LiCoInF6	Na2SiF6	
LiNiInF6	Na2SiF6	
NaCaAlF6	Na2SiF6	
NaMnCrF6	Na2SiF6	
NaMnFeF6	Na2SiF6	
NaMnAlF6	Na2SiF6	
LiMgCrF6	Trirutile	
LiMgGaF6	Trirutile	
LiMgRhF6	Trirutile	
LiNiTiF6	Trirutile	
LiNiVF6	Trirutile	
LiCoCrF6	Trirutile	
LiCuCrF6	Trirutile	
LiZnCrF6	Trirutile	
LiNiFeF6	Trirutile	
LiNiCoF6	Trirutile	
LiZnCoF6	Trirutile	
LiCoGaF6	Trirutile	
LiNiRhF6	Trirutile	
LiCuRhF6	Trirutile	
LiZnRhF6	Trirutile	
LiMgVF6	Trirutile	
LiFeCrF6	Trirutile	
LiCaAlF6	LiCaAlF6	
LiSrAlF6	LiCaAlF6	
LiCaVF6	LiCaAlF6	
LiCaCrF6	LiCaAlF6	
LiCaCoF6	LiCaAlF6	
LiCaRhF6	LiCaAlF6	

Composition	Crystal type	Space group
LiSrTiF6	LiCaAlF6	
LiSrCrF6	LiCaAlF6	
LiCdCrF6	LiCaAlF6	
LiCdFeF6	LiCaAlF6	
LiPbFeF6	LiCaAlF6	
LiCdCoF6	LiCaAlF6	
LiPbGaF6	LiCaAlF6	
LiCdRhF6	LiCaAlF6	
LiCdTiF6	LiCaAlF6	
CsMgAlF6	RbNiCrF6	
CsMgTiF6	RbNiCrF6	
CsMgVF6	RbNiCrF6	
CsMgCrF6	RbNiCrF6	
CsMgFeF6	RbNiCrF6	
TlMgFeF6	RbNiCrF6	
RbMgCoF6	RbNiCrF6	
CsMgGaF6	RbNiCrF6	
RbNiAlF6	RbNiCrF6	
KNiCrF6	RbNiCrF6	
CsPdScF6	RbNiCrF6	
CsCoTiF6	RbNiCrF6	
CsZnTiF6	RbNiCrF6	
CsVMnF6	RbNiCrF6	
RbVFeF6	RbNiCrF6	
CsCoVF6	RbNiCrF6	
CsNiVF6	RbNiCrF6	
CsCuVF6	RbNiCrF6	
CsZnVF6	RbNiCrF6	
CsMnCrF6	RbNiCrF6	
TlMnCrF6	RbNiCrF6	
CsFeCrF6	RbNiCrF6	
TlFeCrF6	RbNiCrF6	
CsCoCrF6	RbNiCrF6	
RbNiCrF6	RbNiCrF6	
TlNiCrF6	RbNiCrF6	
CsCuCrF6	RbNiCrF6	
CsZnCrF6	RbNiCrF6	
CsMnFeF6	RbNiCrF6	
RbZnMnF6	RbNiCrF6	
CsZnMnF6	RbNiCrF6	
CsCoFeF6	RbNiCrF6	
CsNiFeF6	RbNiCrF6	
RbCuFeF6	RbNiCrF6	

Composition	Crystal type	Space group
CsZnFeF6	RbNiCrF6	
RbNiCoF6	RbNiCrF6	
RbCuCoF6	RbNiCrF6	
CsNiGaF6	RbNiCrF6	
CsCuGaF6	RbNiCrF6	
CsCuInF6	RbNiCrF6	
CsCuTlF6	RbNiCrF6	
CsPdRhF6	RbNiCrF6	
CsAgInF6	RbNiCrF6	
CsCuAlF6	CsAgAlF6	
CsZnAlF6	CsAgAlF6	
CsAgAlF6	CsAgAlF6	
CsAgFeF6	CsAgAlF6	
RbAgGaF6	CsAgAlF6	
LiBaVF6		P2(1)/c, Z=4
LiBaCrF6		P2(1)/c, Z=4
LiBaCoF6		P2(1)/c, Z=4
KBeYF6		P2(1)/m, Z=2
KBeEuF6		P2(1)/m, Z=2
KBeGdF6		P2(1)/m, Z=2
KBeDyF6		P2(1)/m, Z=2
KBeTmF6		P2(1)/m, Z=2
KBeYbF6		P2(1)/m, Z=2
NaCaCeF6	UCl3	P6(3)/m, Z=1
NaBaCeF6	UCl3	P6(3)/m, Z=1
KCrMnF6	bronze	P4/mbm, Z=5
KCuCrF6		P2(1)/c, Z=4
KBaCeF6	UCl3	P6(3)/m, Z=1
CsNiMnF6	CsNiMnF6	R3(-)m
LiF-BeF2-CeF3	without compound ABCF6	
KF-BeF2-LaF3	without compound ABCF6	
KF-CuF2-YbF3	without compound ABCF6	
KF-CuF2-LuF3	without compound ABCF6	

Table 3.2

Set for Examination

Composition	Crystal type	Space group
LiMgInF6	Na2SiF6	
LiMnFeF6	Na2SiF6	
LiMnGaF6	Na2SiF6	
LiMnInF6	Na2SiF6	
LiZnInF6	Na2SiF6	
LiCdInF6	Na2SiF6	
LiMgTiF6	Trirutile	
LiMgFeF6	Trirutile	
LiMgCoF6	Trirutile	
LiFeTiF6	Trirutile	
LiCoTiF6	Trirutile	
LiZnTiF6	Trirutile	
LiZnVF6	Trirutile	
LiNiCrF6	Trirutile	
LiFeFeF6	Trirutile	
LiCoFeF6	Trirutile	
LiCuFeF6	Trirutile	
LiZnFeF6	Trirutile	
LiCuCoF6	Trirutile	
LiCoRhF6	Trirutile	
LiNiGaF6	Trirutile	
LiCuGaF6	Trirutile	
LiCaTiF6	LiCaAlF6	
LiCaFeF6	LiCaAlF6	
LiCaGaF6	LiCaAlF6	
LiSrVF6	LiCaAlF6	
LiCdVF6	LiCaAlF6	
LiPbVF6	LiCaAlF6	
LiPbCrF6	LiCaAlF6	
LiSrGaF6	LiCaAlF6	
RbMgAlF6	RbNiCrF6	
RbMgCrF6	RbNiCrF6	
KNiAlF6	RbNiCrF6	
CsNiAlF6	RbNiCrF6	
CsVScF6	RbNiCrF6	
CsAgScF6	RbNiCrF6	
CsNiTiF6	RbNiCrF6	
CsCuTiF6	RbNiCrF6	
CsVCrF6	RbNiCrF6	
CsVFeF6	RbNiCrF6	
RbMnCrF6	RbNiCrF6	

Composition	Crystal type	Space group
RbFeCrF6	RbNiCrF6	
RbCoCrF6	RbNiCrF6	
CsNiCrF6	RbNiCrF6	
RbCuCrF6	RbNiCrF6	
RbZnCrF6	RbNiCrF6	
CsMnGaF6	RbNiCrF6	
RbNiFeF6	RbNiCrF6	
CsCuFeF6	RbNiCrF6	
CsPdFeF6	RbNiCrF6	
CsNiCoF6	RbNiCrF6	
RbZnCoF6	RbNiCrF6	
CsNiInF6	RbNiCrF6	
CsZnInF6	RbNiCrF6	
CsPdInF6	RbNiCrF6	
CsAgTlF6	RbNiCrF6	
RbCuAlF6	CsAgAlF6	
RbAgAlF6	CsAgAlF6	
RbCuVF6	CsAgAlF6	
RbAgFeF6	CsAgAlF6	
CsAgGaF6	CsAgAlF6	
LiBaAlF6		P2(1)/c, Z=4
LiBaTiF6		P2(1)/c, Z=4
LiBaFeF6		P2(1)/c, Z=4
LiBaGaF6		P2(1)/c, Z=4
KBeSmF6		P2(1)/m, Z=2
KBeTbF6		P2(1)/m, Z=2
KBeHoF6		P2(1)/m, Z=2
KBeErF6		P2(1)/m, Z=2
KBeLuF6		P2(1)/m, Z=2
KCaCeF6	UCl3	P6(3)/m, Z=1
KCrFeF6	bronze	P4/mbm, Z=5
KCoFeF6	bronze	P4/mbm, Z=5
RbMnFeF6	NH4MnFeF6	Pb2n
NaF-PbF2-BiF3	without compound ABCF6	
KF-CuF2-BiF3	without compound ABCF6	

In the former case the quantitative properties were quantized on the basis of uniform distribution of the values of the intervals (traditional way). Table 3.3 contains the gradations for Feature Set 3.1. In this case no clear-cut distinction exists between features of flu-

orides with compositions AF_2, BF_3 and CF . Moreover if the feature values for different fluorides (components of the certain physical-chemical system) coinside then either of two values is eliminated from the description of this system.

Table 3.3

Gradations for Feature Set 3.1
(Properties of Simple Fluorides)
(Traditional Way)

Feature	Gradation	Feature	Gradation
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[77-129]	H_1	[9-12.2]	Cp_1
(129-147]	H_2	(12.2-15.7]	Cp_2
(147-167]	H_3	(15.7-16.7]	Cp_3
(167-198]	H_4	(16.7-22]	Cp_4
(198-256]	H_5	Melting point of simple fluorides, K	
(256-292]	H_6	[600-1048]	Tm_1
(292-395]	H_7	(1048-1148]	Tm_2
Standard entropy for corresponding simple fluorides, cal/mol*K		(1148-1300]	Tm_3
		(1300-1430]	Tm_4
		(1430-1550]	Tm_5
		(1550-1700]	Tm_6
[8-15.9]	So_1	Ionic radii, A	
(15.9-18]	So_2	[0.27-0.615]	Rs_1
(18-19.6]	So_3	(0.615-0.665]	Rs_2
(19.6-22.3]	So_4	(0.665-0.74]	Rs_3
(22.3-23.2]	So_5	(0.74--0.76]	Rs_4
(23.2-28]	So_6	(0.76-0.80]	Rs_5
(28-35]	So_7	(0.80-0.94]	Rs_6
		(0.94-1.19]	Rs_7
		(1.19-1.7]	Rs_8

In the latter case the quantitative properties were quantized on the basis of the use of the discretization program. Table 3.4 contains the gradations for Feature Set 3.2.

Table 3.4

Gradations for Feature Set 3.2
(Properties of Simple Fluorides)
(Use of Discretization Program)

Feature	Gradation	Feature	Gradation
	AF		
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[78 -		[9.99 -	
- 82.1346001625061]	H_1_1	- 10.1765999959409]	Cp_1_1
[128.993402004242-		[11.0473999769986-	
- 134.506202220917]	H_2_1	- 11.3583999702334]	Cp_2_1
(134.506202220917-		[11.6071999648213-	
- 135.884402275085]	H_3_1	- 11.8559999594092]	Cp_3_1
(135.884402275085-		[11.9803999567032-	
- 140.019002437592]	H_4_1	- 12.1669999526441]	Cp_4_1
[142.775402545929-		(12.1669999526441-	
- 146.910002708435]	H_5_1	- 12.353599948585]	Cp_5_1
Standard entropy for corresponding simple fluorides, cal/mol*K		Melting point of simple fluorides, K	
		[600 -	
		- 640.079998970032]	Tm_1_1
		[960.719990730286 -	
[8.523 -		- 1080.95998764038]	Tm_2_1
- 9.38382002520561]	So_1_1	[1107.67998695374-	
[11.6793400924206-		- 1268]	Tm_3_1
- 12.8271001260281]	So_2_1	Ionic radii, A	
[15.122620193243-		[0.76 -	
- 16.5573202352524]	So_3_1	- 0.814600002244115]	Rs_1_1
[18.2789602856636-		[0.996600009724498-	
- 19.4267203192711]	So_4_1	- 1.06940001271665]	Rs_2_1
[21.7222403864861-		[1.36060002468526-	
- 22.5830604116917]	So_5_1	- 1.43340002767742]	Rs_3_1
(22.5830604116917-		[1.46980002917349-	
- 22.8700004200935]	So_6_1	- 1.50620003066957]	Rs_4_1
		(1.50620003066957-	
		- 1.56080003291369]	Rs_5_1
		[1.63360003590584-	
		- 1.67000003740192]	Rs_6_1

Feature	Gradation	Feature	Gradation
	BF 2		
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[85.9 -		[12.39 -	
- 98.2540000915527]	H_1_2	- 12.7086000064015]	Cp_1_2
[106.490000152588-		[13.9830000320077-	
- 122.962000274658]	H_2_2	- 14.5140000426769]	Cp_2_2
(122.962000274658-		(14.5140000426769-	
- 139.434000396729]	H_3_2	- 14.9388000512123]	Cp_3_2
[147.670000457764-		[15.15120005548-	
- 160.024000549316]	H_4_2	- 16.0008000725508]	Cp_4_2
(160.024000549316-		(16.0008000725508-	
- 176.496000671387]	H_5_2	- 16.2132000768185]	Cp_5_2
(176.496000671387-		(16.2132000768185-	
- 184.732000732422]	H_6_2	- 16.4256000810862]	Cp_6_2
(184.732000732422-		(16.4256000810862-	
- 197.086000823975]	H_7_2	- 16.6380000853539]	Cp_7_2
(197.086000823975-		(16.6380000853539-	
- 201.204000854492]	H_8_2	- 16.7442000874877]	Cp_8_2
(201.204000854492-		(16.7442000874877-	
- 213.558000946045]	H_9_2	- 16.9566000917554]	Cp_9_2
[238.26600112915-		(16.9566000917554-	
- 254.738001251221]	H_10_2	- 17.2752000981569]	Cp_10_2
[262.974001312256-		[17.4876001024246-	
- 279.446001434326]	H_11_2	- 17.7000001066923]	Cp_11_2
(279.446001434326-		Melting point of simple fluorides, K	
- 287.682001495361]	H_12_2	[970 -	
(287.682001495361-		- 1013.26000022888]	Tm_1_2
- 291.800001525879]	H_13_2	(1013.26000022888-	
Standard entropy for corresponding simple fluorides, cal/mol*K		- 1056.52000045776]	Tm_2_2
		(1056.52000045776-	
		- 1085.36000061035].	Tm_3_2
		(1085.36000061035-	2
[12.75 -		- 1128.62000083923]	Tm_4_2
- 13.6049999892712]	So_1_2	(1128.62000083923-	
(13.6049999892712-		- 1143.04000091553]	Tm_5_2
- 14.4599999785423]	So_2_2	(1143.04000091553-	
[15.5999999642372-		- 1157.46000099182]	Tm_6_2
- 18.4499999284744]	So_3_2	(1157.46000099182-	

Feature	Gradation	Feature	Gradation
(18.4499999284744-		- 1200.7200012207]	Tm_7_2
- 19.5899999141693]	So_4_2	(1200.7200012207-	
(19.5899999141693-		- 1258.40000152588]	Tm_8_2
- 19.874999910593]	So_5_2	[1316.08000183106-	
(19.874999910593-		- 1373.76000213623]	Tm_8_2
- 20.4449999034405]	So_6_2	(1373.76000213623-	
(20.4449999034405-		- 1388.18000221252]	Tm_10_2
- 20.7299998998642]	So_7_2	(1388.18000221252-	
(20.7299998998642-		- 1460.28000259399]	Tm_11_2
- 21.5849998891354]	So_8_2	[1517.96000289917-	
(21.5849998891354-		- 1575.64000320435]	Tm_12_2
- 22.4399998784065]	So_9_2	(1575.64000320435-	
(22.4399998784065-		- 1633.32000350952]	Tm_13_2
- 23.009999871254]	So_10_2	(1633.32000350952-	
(23.009999871254-		- 1676.5800037384]	Tm_14_2
- 27]	So_11_2	(1676.5800037384-	
		- 1691.0000038147]	Tm_15_2
		Ionic radii, A	
		[0.45 -	
		- 0.503999997675419]	Rs_1_2
		[0.647999991476536-	
		- 0.791999985277653]	Rs_2_2
		(0.791999985277653-	
		- 0.827999983727932]	Rs_3_2
		(0.827999983727932-	
		- 0.845999982953072]	Rs_4_2
		(0.845999982953072-	
		- 0.89999998062849]	Rs_5_2
		(0.89999998062849-	
		- 1.04399997442961]	Rs_6_2
		[1.15199996978045-	
		- 1.35]	Rs_7_2
	CF 3		
Standard enthalpy of formation for corresponding simple fluorides, kcal/mol		Standard isobaric thermal capacity for simple fluorides, cal/mol*K	
[175 -		[8.22 -	
- 184.5640001297]	H_1_3	- 18.1701999947429]	Cp_1_3
(184.5640001297-		[18.6105999842286-	
		- 21.62]	Cp_2_3

Feature	Gradation	Feature	Gradation
- 198.910000324249]	H_2_3	Melting point of	
(216 -		simple fluorides, K	
- 246.730000972748]	H_3_3	[823-1000]	Tm_1_3
(246.730000972748-		[1203.76001739502-	
- 251.512001037598]	H_4_3	- 1344.04002380371]	Tm_2_3
(251.512001037598-		(1344.04002380371-	
- 289.768001556397]	H_5_3	- 1404.16002655029]	Tm_3_3
[337.588002204895-		(1404.16002655029-	
- 371.062002658844]	H_6_3	- 1444.24002838135]	Tm_4_3
[380.626002788544-		(1444.24002838135-	
- 390.190002918243]	H_7_3	- 1504.36003112793]	Tm_5_3
(390.190002918243-		(1504.36003112793-	
- 394.972002983093]	H_8_3	- 1544.44003295898]	Tm_6_3
(394.972002983093-		(1544.44003295898-	
- 409.318003177643]	H_9_3	- 1604.56003570557]	Tm_7_3
(409.318003177643-		[1644.64003753662-	
- 414.100003242493]	H_10_3	- 1704.7600402832]	Tm_8_3
Standard entropy		(1704.7600402832-	
for corresponding		- 1764.88004302979]	Tm_9_3
simple fluorides,		(1764.88004302979-	
cal/mol*K		- 1804.96004486084]	Tm_10_3
[15.89 -		(1804.96004486084-	
- 16.9765999758244]	So_1_3	- 1825.00004577637]	Tm_11_3
(16.9765999758244-		Ionic radii, A	
- 17.7009999597073]	So_2_3	[0.535 -	
(17.7009999597073-		- 0.564820000752807]	Rs_1_3
- 18.7875999355316]	So_3_3	[0.584700001254678-	
[20.2363999032974-		- 0.614520002007485]	Rs_2_3
- 22.0473998630047]	So_4_3	(0.614520002007485-	
(22.0473998630047-		- 0.664220003262162]	Rs_3_3
- 23.858399822712]	So_5_3	(0.664220003262162-	
(23.858399822712-		- 0.694040004014969]	Rs_4_3
- 24.9449997985363]	So_6_3	[0.733800005018711-	
(24.9449997985363-		- 0.773560006022453]	Rs_5_3
- 25.6693997824192]	So_7_3	(0.773560006022453-	
(25.6693997824192-		- 0.823260007277131]	Rs_6_3
- 26.3937997663021]	So_8_3	[0.843140007779002-	
(26.3937997663021-		- 0.863020008280873]	Rs_7_3
- 27.4803997421265]	So_9_3	(0.863020008280873-	
(27.4803997421265-		- 0.872960008531809]	Rs_8_3
- 27.8425997340679]	So_10_3	(0.872960008531809-	
(27.8425997340679-		- 0.882900008782744]	Rs_9_3
- 28.9291997098923]	So_11_3	(0.882900008782744-	

Feature	Gradation	Feature	Gradation
(28.9291997098923-		- 0.89284000903368]	Rs_10_3
- 30.0157996857166]	So_12_3	(0.89284000903368-	
[32.9133996212483-		- 0.972360011041164]	Rs_11_3
- 58.32]	So_13_3	[0.992240011543036-	
		- 1.02206001229584]	Rs_12_3
		(1.02206001229584-	
		- 1.03200001254678]	Rs_13_3

The Table 3.5 contains the results of examination recognition using the traditional way of the feature discretization.

Table 3.5

Results of Examination
(Traditional Way)

Composition	Crystal type	Result of examination
LiMgInF6	Na2SiF6	Na2SiF6
LiMnFeF6	Na2SiF6	?
LiMnGaF6	Na2SiF6	?
LiMnInF6	Na2SiF6	Na2SiF6
LiZnInF6	Na2SiF6	Na2SiF6
LiCdInF6	Na2SiF6	Na2SiF6
LiMgTiF6	Trirutile	LiCaAlF6
LiMgFeF6	Trirutile	Trirutile
LiMgCoF6	Trirutile	?
LiFeTiF6	Trirutile	LiCaAlF6
LiCoTiF6	Trirutile	LiCaAlF6
LiZnTiF6	Trirutile	LiCaAlF6
LiZnVF6	Trirutile	Trirutile
LiNiCrF6	Trirutile	?
LiFeFeF6	Trirutile	Na2SiF6
LiCoFeF6	Trirutile	Trirutile
LiCuFeF6	Trirutile	?
LiZnFeF6	Trirutile	?
LiCuCoF6	Trirutile	?
LiCoRhF6	Trirutile	LiCaAlF6
LiNiGaF6	Trirutile	Trirutile
LiCuGaF6	Trirutile	?
LiCaTiF6	LiCaAlF6	LiCaAlF6
LiCaFeF6	LiCaAlF6	LiCaAlF6
LiCaGaF6	LiCaAlF6	LiCaAlF6
LiSrVF6	LiCaAlF6	LiCaAlF6

Composition	Crystal type	Result of examination
LiCdVF6	LiCaAlF6	LiCaAlF6
LiPbVF6	LiCaAlF6	LiCaAlF6
LiPbCrF6	LiCaAlF6	?
LiSrGaF6	LiCaAlF6	LiCaAlF6
RbMgAlF6	RbNiCrF6	RbNiCrF6
RbMgCrF6	RbNiCrF6	?
KNiAlF6	RbNiCrF6	?
CsNiAlF6	RbNiCrF6	RbNiCrF6
CsVScF6	RbNiCrF6	RbNiCrF6
CsAgScF6	RbNiCrF6	CsAgAlF6
CsNiTiF6	RbNiCrF6	RbNiCrF6
CsCuTiF6	RbNiCrF6	CsAgAlF6
CsVCrF6	RbNiCrF6	?
CsVFeF6	RbNiCrF6	CsAgAlF6
RbMnCrF6	RbNiCrF6	?
RbFeCrF6	RbNiCrF6	CsAgAlF6
RbCoCrF6	RbNiCrF6	?
CsNiCrF6	RbNiCrF6	?
RbCuCrF6	RbNiCrF6	?
RbZnCrF6	RbNiCrF6	?
CsMnGaF6	RbNiCrF6	RbNiCrF6
RbNiFeF6	RbNiCrF6	RbNiCrF6
CsCuFeF6	RbNiCrF6	RbNiCrF6
CsPdFeF6	RbNiCrF6	CsAgAlF6
CsNiCoF6	RbNiCrF6	RbNiCrF6
RbZnCoF6	RbNiCrF6	?
CsNiInF6	RbNiCrF6	RbNiCrF6
CsZnInF6	RbNiCrF6	?
CsPdInF6	RbNiCrF6	?
CsAgTlF6	RbNiCrF6	CsAgAlF6
RbCuAlF6	CsAgAlF6	?
RbAgAlF6	CsAgAlF6	?
RbCuVF6	CsAgAlF6	RbNiCrF6
RbAgFeF6	CsAgAlF6	CsAgAlF6
CsAgGaF6	CsAgAlF6	CsAgAlF6
LiBaAlF6	another structure	?
LiBaTiF6	another structure	?
LiBaFeF6	another structure	?
LiBaGaF6	another structure	?
KBeSmF6	another structure	another structure
KBeTbF6	another structure	another structure
KBeHoF6	another structure	another structure
KBeErF6	another structure	another structure

Composition	Crystal type	Result of examination
KBeLuF6	another structure	another structure
KCaCeF6	another structure	without compound ABCF6
KCrFeF6	another structure	another structure
KCoFeF6	another structure	without compound ABCF6
RbMnFeF6	another structure	?
NaF-PbF2-BiF3	without compound ABCF6	LiCaAlF6
KF-CuF2-BiF3	without compound ABCF6	?

The Table 3.6 contains results of examination recognition after the use of discretization program.

Table 3.6

Results of Examination
(After Use of Discretization Program)

Composition	Crystal type	Result of examination
LiMgInF6	Na2SiF6	?
LiMnFeF6	Na2SiF6	?
LiMnGaF6	Na2SiF6	?
LiMnInF6	Na2SiF6	?
LiZnInF6	Na2SiF6	?
LiCdInF6	Na2SiF6	?
LiMgTiF6	Trirutile	Trirutile
LiMgFeF6	Trirutile	?
LiMgCoF6	Trirutile	Trirutile
LiFeTiF6	Trirutile	Trirutile
LiCoTiF6	Trirutile	Trirutile
LiZnTiF6	Trirutile	Trirutile
LiZnVF6	Trirutile	?
LiNiCrF6	Trirutile	Trirutile
LiFeFeF6	Trirutile	?
LiCoFeF6	Trirutile	?
LiCuFeF6	Trirutile	?
LiZnFeF6	Trirutile	?
LiCuCoF6	Trirutile	Trirutile
LiCoRhF6	Trirutile	Trirutile
LiNiGaF6	Trirutile	Trirutile
LiCuGaF6	Trirutile	Trirutile
LiCaTiF6	LiCaAlF6	Trirutile
LiCaFeF6	LiCaAlF6	?
LiCaGaF6	LiCaAlF6	?

Composition	Crystal type	Result of examination
LiSrVF6	LiCaAlF6	?
LiCdVF6	LiCaAlF6	LiCaAlF6
LiPbVF6	LiCaAlF6	?
LiPbCrF6	LiCaAlF6	?
LiSrGaF6	LiCaAlF6	?
RbMgAlF6	RbNiCrF6	RbNiCrF6
RbMgCrF6	RbNiCrF6	RbNiCrF6
KNiAlF6	RbNiCrF6	without compound ABCF6
CsNiAlF6	RbNiCrF6	RbNiCrF6
CsVScF6	RbNiCrF6	RbNiCrF6
CsAgScF6	RbNiCrF6	RbNiCrF6
CsNiTiF6	RbNiCrF6	RbNiCrF6
CsCuTiF6	RbNiCrF6	RbNiCrF6
CsVCrF6	RbNiCrF6	RbNiCrF6
CsVFeF6	RbNiCrF6	RbNiCrF6
RbMnCrF6	RbNiCrF6	?
RbFeCrF6	RbNiCrF6	?
RbCoCrF6	RbNiCrF6	RbNiCrF6
CsNiCrF6	RbNiCrF6	RbNiCrF6
RbCuCrF6	RbNiCrF6	RbNiCrF6
RbZnCrF6	RbNiCrF6	RbNiCrF6
CsMnGaF6	RbNiCrF6	?
RbNiFeF6	RbNiCrF6	RbNiCrF6
CsCuFeF6	RbNiCrF6	RbNiCrF6
CsPdFeF6	RbNiCrF6	RbNiCrF6
CsNiCoF6	RbNiCrF6	RbNiCrF6
RbZnCoF6	RbNiCrF6	RbNiCrF6
CsNiInF6	RbNiCrF6	RbNiCrF6
CsZnInF6	RbNiCrF6	RbNiCrF6
CsPdInF6	RbNiCrF6	RbNiCrF6
CsAgTlF6	RbNiCrF6	RbNiCrF6
RbCuAlF6	CsAgAlF6	RbNiCrF6
RbAgAlF6	CsAgAlF6	RbNiCrF6
RbCuVF6	CsAgAlF6	RbNiCrF6
RbAgFeF6	CsAgAlF6	RbNiCrF6
CsAgGaF6	CsAgAlF6	?
LiBaAlF6	another structure	?
LiBaTiF6	another structure	Trirutile
LiBaFeF6	another structure	?
LiBaGaF6	another structure	?
KBeSmF6	another structure	another structure
KBeTbF6	another structure	another structure
KBeHoF6	another structure	another structure

Composition	Crystal type	Result of examination
KBeErF6	another structure	another structure
KBeLuF6	another structure	another structure
KCaCeF6	another structure	without compound ABCF6
KCrFeF6	another structure	?
KCoFeF6	another structure	?
RbMnFeF6	another structure	RbNiCrF6
NaF-PbF2-BiF3	without compound ABCF6	Na2SiF6
KF-CuF2-BiF3	without compound ABCF6	without compound ABCF6

The Table 3.7 contains the comparison of results for both ways. The analysis of this Table and Tables 3.5 and 3.6 shows that the use of discretization program improves results to a marked degree.

Table 3.7

Estimation of Results of Examination

	Traditional Way	Discretization Program
Class of Na2SiF6:		
number of objects	6	6
correctly	4 [66.666667 %]	0 [0 %]
incorrectly	0 [0 %]	0 [0 %]
indeterminately	2 [33.333333 %]	6 [100 %]
Class of trirutile :		
number of objects	16	16
correctly	4 [25 %]	10 [62.5 %]
incorrectly	6 [37.5 %]	0 [0 %]
indeterminately	6 [37.5 %]	6 [37.5 %]
Class of LiCaAlF6 :		
number of objects	8	8
correctly	7 [87.5 %]	1 [12.5 %]
incorrectly	0 [0 %]	1 [12.5 %]
indeterminately	1 [12.5 %]	6 [75 %]
Class of RbNiCrF6 :		
number of objects	26	26
correctly	9 [34.615385 %]	22 [84.615385 %]
incorrectly	6 [23.076923 %]	1 [3.8461538 %]
indeterminately	11 [42.307692 %]	3 [11.538462 %]

	Traditional Way	Discretization Program
Class of CsAgAlF6 :		
number of objects	5	5
correctly	2 [40 %]	0 [0 %]
incorrectly	1 [20 %]	4 [80 %]
indeterminately	2 [40 %]	1 [20 %]
Class of another structure:		
number of objects	13	13
correctly	6 [46.153846 %]	5 [38.461538 %]
incorrectly	2 [15.384615 %]	3 [23.076923 %]
indeterminately	5 [38.461538 %]	5 [38.461538 %]
Class of without_compound :		
number of objects	2	2
correctly	0 [0 %]	1 [50 %]
incorrectly	1 [50 %]	1 [50 %]
indeterminately	1 [50 %]	0 [0 %]
Number of objects	76	76
correctly	32 [42.105263 %]	39 [51.315789 %]
incorrectly	16 [21.052632 %]	10 [13.157895 %]
indeterminately	28 [36.842105 %]	27 [35.526316 %]

4. DISCUSSION

4.1. CRYSTAL STRUCTURE AND ELECTRO-OPTICAL PROPERTIES

Only the noncentrosymmetric (acentric) phases have linear EO, nonlinear-optical and piezoelectric properties. The potential EO crystals must contain easily deformable atomic frames (e.g., pyramids, tetrahedra, distorted octahedra, and their combinations) [9]. The structure must be incoherent. The examples of such structures - langbeinites, melilites, weberites, hantites, colquirites, and other potential crystals which were predicted in this investigation. The new EO compounds should be searched among families containing the known EO substances for. The predicted crystal structure types do not exhaust the list of promissing compounds. Problem is connected with volume of information for computer learning.

4.2. DB AND PREDICTION OF INORGANIC COMPOUNDS WITH PREDEFINED PROPERTIES

The experience of prediction of new inorganic compounds gives grounds that only databases (DB) can provide with sufficient volume and representativeness of the learning set. In this case the system of the artificial intelligence is a mean for processing large information bulks of DBs on substance and material properties. The goal of this processing is a search for regularities in data and an use of there regularities for the prediction of the possibility of forming inorganic compounds and the estimation of their properties.

The developed by us databases containing ternary compound properties [35,36], the properties of crystals of acousto-optical, electro-optical, and nonlinear-optical materials [37-39] can be used for the search information for the computer learning.

The integration of DB and predicting systems, based on the principles of artificial intelligence, is a tendency of the inorganic compounds computer design. The information-predicting system, that we develop [40-42], is a practical realization of such an approach. A necessary condition of further investigations, connected with prediction of new EO compounds, is development of the specialized system of this kind for the EO material applications.

4.3. PROGRAM OF DISCRETIZATION: EXPERIENCE OF THE USE AND PERSPECTIVES OF IMPROVEMENT

Application of computer discretization allowed to raise the accuracy of prediction, reduce calculation time and laboriouness of preprocessing. But the possibility exists of improvement of this program.

Firstly, the program must take into account the isolated objects which do not follow the main object distribution. For example, majority of compounds with composition $LiMgCF_6$ have crystal structure of trirutile but only $LiMgAlF_6$ and $LiMgInF_6$ have Na_2SiF_6 crystal structure at normal state. But the all unknown compounds $LiBCF_6$ were predicted as having trirutile crystal structure. Is it correct - this is possible to test only by experiment. I such a situation the weight of object for computer learning must be taken into account. This weight must be assessed by expert.

Secondly, it is essential that the features can be some algebraic

function of several component properties. For example, $F = (r_A + r_B)/2$, where r_A and r_B - ionic radii of elements A and B. Such features will divide the classes better. The problem is only one of computer discretization of such complicated features for both learning set and set for prediction.

4.4. SEARCH FOR POLYFUNCTIONAL MATERIALS

It is significant that predicted compounds are able to be polyfunctional materials because they can have not only EO but also nonlinear-optical, piezo-electric, ferroelectric and other properties. The application of polyfunctional materials is a tendency of development of devices for integrated electronics [2]. In this case it is necessary to predict the compounds which hold the promise for searching for new electro-optical, nonlinear-optical, acousto-optical, laser, and other materials in various combinations.

4.5. COMBINATION OF AI WITH OTHER THEORETICAL METHODS

The necessity of fulfilment of the condition of compactness for compounds classes in the chemical elements' properties multi-dimensional space is a peculiarity of computer learning application. I.e., only the qualitative leap of predicted property can ensure a good division of objects of different classes. It is impossible to divide the objects whose target property has a form of linear dependence. In the latter simple case it is pertinent to use any algebraic equation (for example, regression dependence). Computer learning is a powerful tool of searching for complicated regularities but naturally it is not an universal mean for solution of the all chemical problems. It has its application area connected with prediction of belonging to some discrete class. Only combination of computer learning with other calculation methods will allow to solve various chemical problems.

5. CONCLUSIONS

1. The prediction of the crystal structure types (langbeinite or $K_2Zn_2(MoO_4)_3$) at normal pressure and room temperature for the new compounds with composition of $A_2^{I}B_2^{II}(X_4O_3)_3^{VI}$ (A and B - any chemical elements; X - S, Cr, Mo, or W) is carried out. The great number of predicted compounds with langbeinite structure hold the promise for searching for new EO materials.

2. Prediction of the melilite crystal structure types at standard condiditions for the compounds with compositions $A^{II}_2 B^{II}_2 X^{IV} O_7$ (A and B - any chemical elements; X - Si, Ge, Sn, Ti, Zr, or Hf) and $A^{II}_2 X^{IV} B^{III}_2 O_7$ (A and B - any chemical elements; X - Si, Ge or Ti) was also carried out. Analysis of results shows: the great number of predictions of new melilites were obtained which hold the promise for searching for new EO materials.

3. The results of predicting the crystal structure types (hantite, calcite or aragonite) at normal pressure and room temperature for the complicated borates with composition of $AD(BO_3)_4$ (A and D - any chemical elements; B - boron) are presented. Only compounds with acentric crystal structure type of hantite hold the promise for searching for new EO materials.

4. For composition $A^{I} B^{II} C^{III} F_6$ (A = Li, Na, K, Rb, or Cs; B and C - any chemical elements) types considered included: trirutile, colquirite ($LiCaAlF_6$), Na_2SiF_6, $RbNiCrF_6$, and $CsAgFeF_6$. Analysis of results shows: the great number of predictions of new compounds with colquirite acentric crystal structure types and Na_2SiF_6 were obtained, which hold the promise for searching for new EO materials.

5. Prediction of the crystal structure types (orthorhombic and trigonal weberites and fluorite) at standard conditions for the new compounds with composition $A^{I}_2 B^{II} C^{III} F_7$ (A - Na or Ag; B and C - any chemical elements) was also carried out. Analysis of results shows that many new compounds with crystal structure type of orthorhombic and trigonal weberites, which hold the promise for searching for new EO materials, were obtained.

6. The efficiency of the use of discretization program was shown on the base of testing certain task.

7. The ways of improvement of computer learning methods were discussed (use of DBs, additions to discretization program, design of comp-

licated component features, etc.).

8. Next goal to be sought is a prediction of polyfuntional materials for development of integrated electronic devices.

9. The possibilities of combination of computer learning with other calculation methods were discussed. This way will allow to solve the more wide class of chemical and materials science problems.

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